Agilent ChemStation Plus

XML Connectivity Guide

Agilent Technologies

Notices

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Manual Part Number

G2170-90223

Edition

05/2005 Printed in Germany

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This guide is valid for B.01.xx revisions of the Agilent ChemStation Plus software, where xx refers to minor revisions of the software that do not affect the technical accuracy of this guide.

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In This Guide...

This guide contains installation and reference information for the XML interface between the Agilent ChemStation and a LIMS system. The Appendixes contain examples of the XML files and the schemas used to generate them.

NOTE Running XML using ChemStation Rev. A.10.x and ChemStore Rev. B.03.01 this manual is not applicable. Please refer to the appropriate *XML Interface Guide* in the manual section of your Rev. B.03.0x ChemStore CD-ROM.

1 XML in the Agilent ChemStation

This chapter gives an introduction to XML, and describes how the interface is implemented.

2 Enabling XML Functionality

In this chapter, the changes that have to be made to enable the XML interface functions in the Agilent ChemStation are described.

3 Import Worklist

This chapter contains an explanation of how the Agilent ChemStation imports an XML file from the LIMS system.

4 LIMS Fields: Linking the Sample to the Result File

This chapter describes how the samples and their associated data are uniquely identified in the XML interface.

5 Export Data

This chapter explains how the Agilent ChemStation exports the XML file to the LIMS system.

6 XML in Agilent ChemStore

This chapter explains how to use the previously described XML for Agilent ChemStation in conjunction with Agilent ChemStore. It shows how the workflow differs from

ChemStation and the different Oracle tables & views that are used. Additionally, this chapter explains the changes that have to be made to enable the XML interface functions in the Agilent ChemStation to allow it to work with ChemStore and how to import a work list.

7 ChemStore for LIMS interfacing

This chapter describes the configuration of ChemStore to allow the export of runs to LIMS.

8 LIMS ORACLE Views and Tables within ChemStore and extacting their data

This chapter describes the contents of Oracle Views and tables used for storage of information which can be used by a LIMS system to extract the required data.

9 Generic XML based Archive/Restore interface between ChemStore and an Archive or Data Management System (DMS)

This chapter defines the concept employed in creating a link between ChemStore and any Archive or Data Management System (DMS) for managing archives from a ChemStore client-server system for long-term storage. This concept employs the Archival and Restore of data by the use of the XML based Archive/Restore Interface. Additionally, this chapter details the flow of data for restoration of information; this process is an interactive process using both the DMS and the ChemStore application to ensure that files are correctly restored to their original location.

10 Installation & Configuration

The chapter details the installation and configuration of the XML-based Archive/Restore plug-in.

11 XML Schema Definition (XSD) for Archive Catalogue File

This chapter describes the generic structure of the XML catalog file generated by the ChemStore Archiver.

A Example Result File

This appendix contains an example of a results file in XML format in the form that would be exported to a LIMS system.

B Export File Schema (EXPORT.XSD)

In this appendix, the schema that is used to produce the results file for export is listed.

C Sample Worklist File

This appendix gives an example of a worklist file of the type that would be imported into the Agilent ChemStation.

D Worklist Schema (WORKLIST.XSD)

This appendix lists the schema that is used to produce the worklist XML file.

E XSD File (XMLSchema.xsd)

This appendix lists the schema that is used to produce a catalog file generated by ChemStore.

F Example XML file (XMLSchema_example.xml)

This appendix shows an example XML file.

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This chapter gives an introduction to XML, and describes how the interface is implemented.

What is XML?

XML (eXtensible Markup Language) is a protocol for structuring data in pure text format; the XML file contains data with embedded structural information and, being pure text, it can be edited with a simple editor like Notepad. XML has become a very flexible and portable format especially for exchanging data between different systems.

XML in the Agilent ChemStation

Because of its flexibility and portability, XML can provide the interconnectivity between the Agilent ChemStation and a LIMS system. The workflow that describes the connectivity can be divided into the five sequential activities shown in Figure 1:

1. the sample list is generated by the LIMS system in an XML format
2. it is imported by the Agilent Chemstation
3. samples are analyzed
4. the results of the analysis are exported to an XML results file
5. the XML results file is transferred back to the LIMS system (manually or automatically)

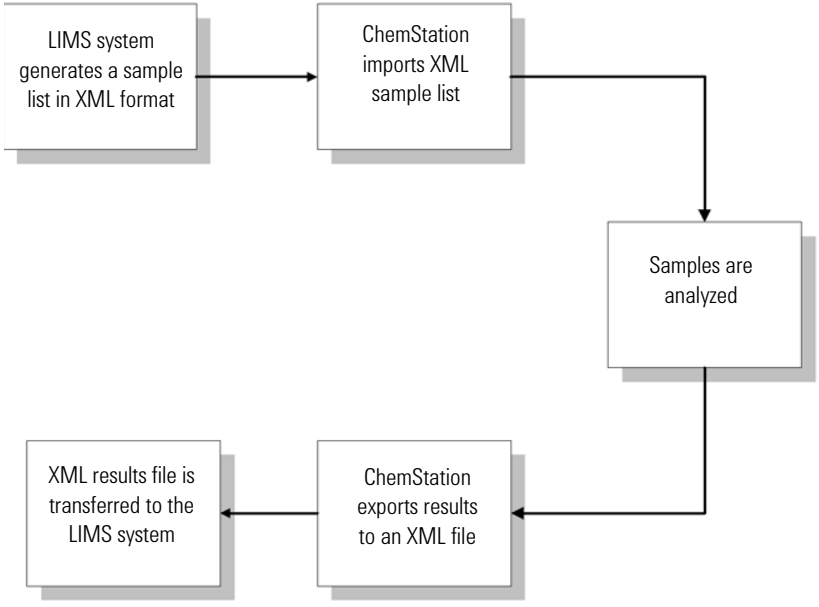
LIMS system generates a sample list in XML format
ChemStation imports XML sample list
Samples are analyzed
ChemStation exports results to an XML file
XML results file is transferred to the LIMS system

Figure 1 Workflow for XML in the Agilent ChemStation

The Agilent ChemStation XML interface manages two tasks:

- import a worklist containing a sequence in XML format
- export a result file in XML format either manually or automatically

Agilent ChemStation XML support uses XSD templates to describe the document schemas.

2
Enabling XML Functionality

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Making Entries in the ini-File

XML functionality in the Agilent ChemStation is enabled by entries in ChemStation-related sections of the CHEMSTATION.INI file. The file is loacted in the windows directory; c:\WINDOWS. Two entries in the [PCS] section of the CHEMSTATION.INI file enable the complete XML export/import functionality. These entries are not written to the CHEMSTATION.INI file during installation, but must be added manually by the system administrator.

[PCS]

XMLEnableImport=1

XMLEnableExport=1

The lack of the entry, or *entry=0* turns off the functionality.

Import-related entries

In the section for each instrument, [PCS,n], a variable specifies the default directory for importing files. This is the directory in which the import file dialog opens, and where the manual import function looks for a file with no specified path.

[PCS,n]

XMLImportPath$=d:\xml\wrkl

Export-related entries

Instrument-specific entries ([PCS,n] section)

[PCS,n]

XMLExportDestUNC$=\\server\share\directory

XMLExportDestUNC$ describes a path to a remote directory to which the result files will be copied when AUTOMATION mode is enabled. It can be a UNC path.

System-specific entries ([PCS] section)

[PCS]

XMLAutomation=1

XMLAutomation enables the AUTOMATION mode, in which the XML results file is copied automatically from the local raw datafile directory to a remote location during the running of a sequence with Data Analysis.

[PCS]

XMLExportCopyWaitTime=3

XMLExportCopyTries=10

XMLExportCopyTries and *XMLExportCopyWaitTime* specify the number of times the copying application tries to copy the results file to a remote location (*XMLExportDestUNC$*), and the time (in seconds) it should wait between successive tries.

[PCS]

XMLExportLocalRecovPath$=c:\Chem32\recovery

When all the tries of copying fail, *XMLExportLocalRecovPath$* specifies the recovery directory to which the XML file is copied. This must be a local directory.

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The XML-formatted worklist is imported into Chemstation as a sequence table. Two modes of import are provided:

- manual/interactive: a menu item allows the user to select the file to be imported
- automatic: a macro function is used to import the file.

General

The XML file is transformed into an intermediate format using an XSL stylesheet and an external application, which uses Windows MSXML libraries for the transformation.

The application needs a Windows MSXML library of version 3.0 or later. Earlier versions of the library, which do not support XSL transformation, must be updated to the newer version. Updates are readily available for free download from the Microsoft web site.

NOTE

It is possible to run \Chem32\SYS\ XML2CSV.EXE from the command line without any parameters. The first line of the output *"Agilent (R) XML Transformer - using MSXML library version 3.0"* specifies the currently used MSXML version.

Format of the worklist file

The worklist file is an XML file formatted as defined by an XML schema file. The schema file describes the structure of the worklist and may be used as a template for creating correct worklist files. The XML schema for worklists to import is stored as "\Chem32\CORE\worklist.xsd". The complete schema is shown in Appendix D. An example XML worklist file is shown in Appendix C.

In general, the XML worklist supports all the fields of the standard sequence table and also the ChemStore Study and ChemStore Custom Fields. It does not support Analyst software Compounds columns. The connectivity between the LIMS systems and Agilent ChemStation software has been achieved by introducing three additional columns: LimsID, LimsKField2 and LimsKField3. These are described in detail in "Cerity Worklist Import – names compatibility" on page 31.

Manual/Interactive import

Sequence Menu

An additional item, Import XML Worklist, appears in the Sequence menu (full menus) in the Method and Run Control view (see Figure 2). The menu item appears only when *XMLEnableImport=1*.

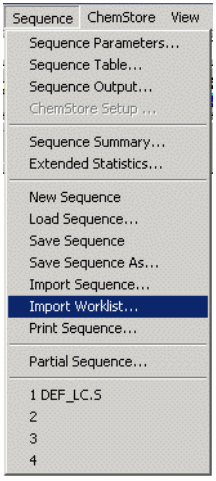

Figure 2 Sequence menu with XML Import

Import XML Worklist displays the Import XML File dialog box (see Figure 3 on page 23), which allows the user to select an XML-formatted worklist to import. The default directory for each instrument is specified separately in the relevant [PCS,n] section of CHEMSTATION.INI. If the variable is not properly specified, or not specified at all, the default directory is _EXEPATH$.

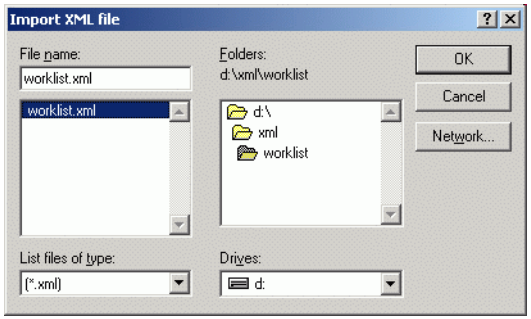

Figure 3 The Import XML File dialog box

XML Import table

If the file has been read successfully, the XML Import table is displayed (see Figure 4 on page 24). It presents a preview of the rows to import. It does not show all fields comprising the worklist, but shows the following columns:

- Line Number
- Vial
- Sample Name
- Method
- Sample Type
- Sample Info
- LimsID
- Study (shown only if the Agilent ChemStation is connected to a Chemstore database).

The window is not resizable; the first three columns are fixed, the horizontal scroll bar allows access to columns at the right of the table.

At this level, no error checking is provided. The table shows all strings as they are, without interpretation. It is the user's responsibility to discard obviously invalid rows.

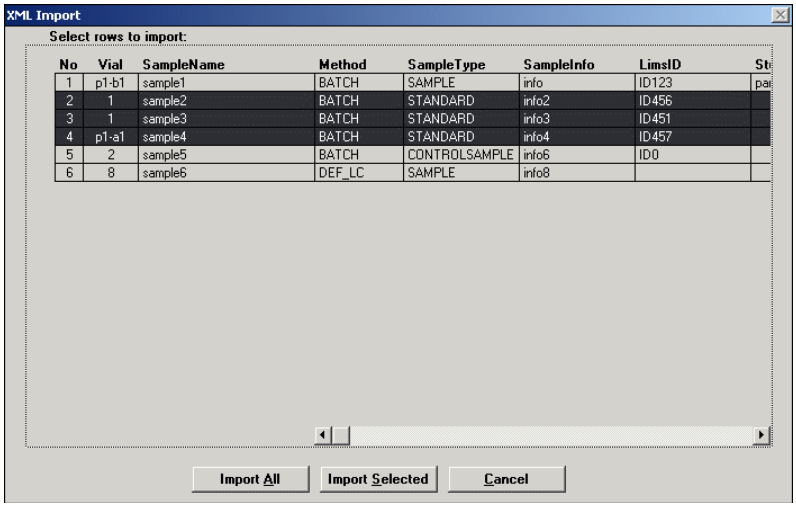
XML Import
Select rows to import:
No Vial SampleName Method SampleType SampleInfo LimsID
1 p1-b1 sample1 BATCH SAMPLE info ID123
2 1 sample2 BATCH STANDARD info2 ID456
3 1 sample3 BATCH STANDARD info3 ID451
4 p1-a1 sample4 BATCH STANDARD info4 ID457
5 2 sample5 BATCH CONTROLSAMPLE info6 ID0
6 8 sample6 DEF_LC SAMPLE info8
Import All
Import Selected
Cancel

Figure 4 The XML Import Table

Selection of multiple rows is possible. The buttons give possibilities to **Import All** rows, **Import Selected** rows and to **Cancel** the import process.

Import process

The interactive import always works in *replace* mode: it replaces the current sequence table with the imported one. All the fields are imported in accordance with Import Sequence rules. Three additional columns are inserted into the current sequence table: LimsID, LimsKField2 and LimsKField3. They are string columns with the maximum size of 40 characters. The corresponding values are imported from the XML worklist input file.

All the columns are checked for correctness but are always imported (even with errors, as Import Sequence does). It is the user's responsibility to make a decision if the worklist should be imported, based on the information shown in the Import Summary (see Figure 5 on page 26).

The columns imported are:

- Location
- Sample Name
- Method
- Number Of Injections
- SampleType
- Cal Level
- Update RF
- Update RT
- Interval
- Sample Amount
- ISTD Amount
- Multiplier
- Dilution
- Data Filename
- Injection Volume
- Sample Info
- Study Name
- LimsID, LimsKField2, LimsKField3
- ChemStore Custom Fields

Import Summary

The Import Summary dialog box works the same way as in Import Sequence. As the import progresses, it shows the current status of the process, and all the errors encountered. The dialog box buttons are inactive until the import is finished.

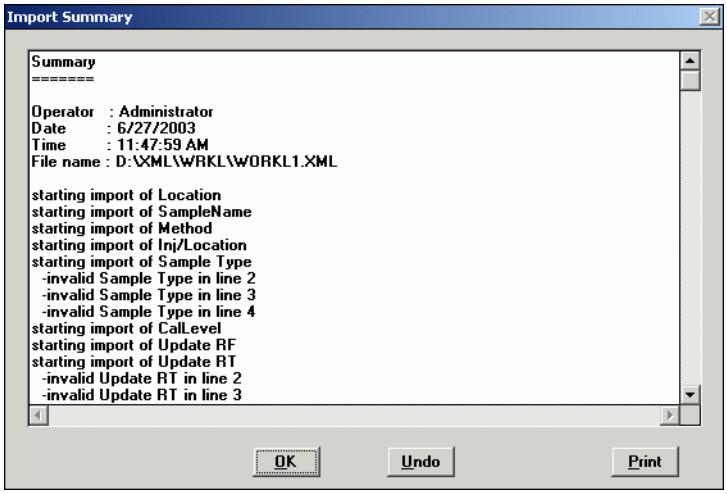

Figure 5 The Import Summary

When the import is complete, the imported sequence table is still a temporary one, and the user has the possibility of confirming the import. The **OK** button exchanges the current sequence table for the imported one; **UNDO** abandons the whole process (the current sequence table remains unchanged); **PRINT** prints the content of the window.

If the input XML file is wrongly formatted, or contains no data, the message **Nothing imported!** is displayed. In this case, both the **OK** and **UNDO** buttons simply close the dialog box, and the current sequence table remains unchanged.

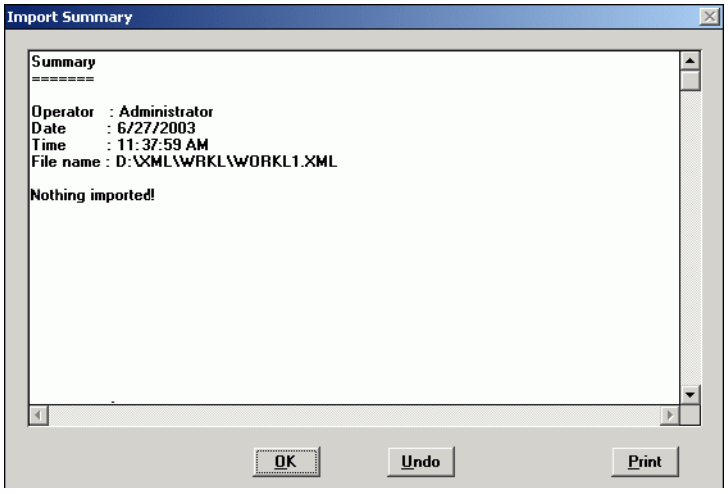

Figure 6 The Import Summary with no import

Automated import

Automated import enables non-interactive import of an XML worklist to the current sequence table. It can be used in any batch process when no interaction is needed or indeed when any interaction is unwelcome.

The macro function that imports the worklist uses the following parameters:

Name XML_ImportWorklist

Parameter ImportFileName$

Parameter boErrorEnds default 0

Parameter boAppendSequence default 0

Parameter boRowSelection default 0

Parameter boSumLog default 0

ImportFileName$

A string describing the full path to the XML worklist to import. If no full path is given, the file is searched in the default XMLImportPath$ directory.

boErrorEnds

A 0/1 variable. 0 is the default setting; the import is not stopped by an error; every value gets imported, even when incorrect, and only the notifications are shown in the summary. 1 stops the import function when it encounters an error.

boAppendSequence

A 0/1 variable. 0 is the default *replace* state. 1 switches to *append* mode, in which the imported data is appended to the current sequence table.

CAUTION The maximum number of rows in the sequence table is 999. Any rows that exceed this number are not imported.

boRowSelection

A 0/1 variable. 0 is the default setting, which disables row selection in the import table, as described in "XML Import table" on page 23. 1 enables interactive row selection.

boSumLog

A 0/1 variable. 0 is the default setting, which suppresses the Import Summary: no summary is produced after having the rows imported, and there is no possibility to undo the import. 1 enables the Import Summary.

The return value describes the last encountered error (when in "boErrorEnds=0" mode) or the error causing the import to stop (when in "boErrorEnds=1" mode). The error code is a combined float value, where the integer part indicates the error type and the fractional part indicates the row number where the error occurred.

Error codes:

0 – no error

1 - wrong type

2 - exceeds the max length

3 - out of range

4 - invalid chars

5 - invalid value

6 - file doesn't exist

7 - seq is running

8 - XML file in invalid format

The error value 2.34 describes that some value in the 34th row exceeded the maximum length limit.

The most frequently used form of the command may look like this:

Val = XML_ImportWorklist(“worklist.xml”)

This imports the file from the default import directory, does not stop on any error, replaces the current sequence table, does not show row selection and suppresses the Import Summary.

Cerity Worklist Import – names compatibility

Table 1 Cerity Worklist Import – names compatibility

Sequence table column	Chemstation XML import field name	Cerity XML import field name
Sequence table	<Samples>	<Samples>
Sequence line	<Sample>	<Sample>
Location	<Location>	
Sample Name	<Name>	<Name>
Method Name	<CDSMethod>	<CDSMethod>
Inj/Location	<numberOfInj>	<numberOfInj>
Sample Type	<sampleType>	<sampleType>
CalLevel	<CalLevel>	(attribute LEVEL of <calibration>)
UpdateRF	<calibration>	(attribute TYPE of <calibration>)
UpdateRT	<UpdateRT>	
Interval	<Interval>	
SampleAmount	<sampleAmount>	<sampleAmount>
Multiplier	<Multipliers>	<Multipliers>/<Multiplier> (a number element)
Dilution	<Dilution>	
Datafile	<Datafile>	
InjVolume	<InjectionVolume>	
Sample Info	<description>	<description>
LimsKField1 (LimsID in editor)	<LimsID>	<LimsID>
LimsKField2	<LimsKField2>	
LimsKField3	<LimsKField3>	

Table 1 Cerity Worklist Import – names compatibility (continued)

Sequence table column	Chemstation XML import field name	Cerity XML import field name
Study	<StudyName>	
Custom Field	<CustomField>/<Name> <CustomField>/<Value>	

4
LIMS Fields: Linking the Sample to the Result File

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One of the main objectives of the implementation of the XML import/export mechanism is the continuity of sample identity in the flow of data between the Agilent ChemStation and the LIMS system. This chapter describes how the samples and their associated data are uniquely identified in the XML interface.

Workflow

The XML import/export function can be envisaged as four separate sub-tasks:

1. The user exports a worklist from a LIMS system.
2. The worklist is imported into the Agilent ChemStation's sequence table
3. Every sample of the worklist is analyzed by the Agilent ChemStation
4. The result datafile is exported back to LIMS system

The main issue is to establish a correspondence between the imported sample information in the worklist and the results exported to the LIMS.

LIMS IDs and a sequence table

"Import process" on page 24 contains a list of the imported columns. Three new columns are introduced: LimsID, LimsKField2 and LimsKField3. Every sample in the worklist may contain additional data in these three fields. The fields can be used, for example, to unambiguously identify the samples in the LIMS system, or for any other LIMS-related purpose.

When the worklist is imported, three additional fixed-length string columns are created in the first sequence table (SeqTable1) of the _SEQUENCE registry. They are given the names of the fields in the worklist: LimsKField1 (displayed as LimsID), LimsKField2 and LimsKField3. For every imported sequence line, appropriate values for the LIMS fields are imported into the sequence table.

Sequence table editor change

The first of the three new fields is shown in a sequence table editor as the LimsID column. It is the last fixed column of the sequence table editor. Analyst-specific columns are placed next to it. It becomes an integral part of the editor and is always visible. When the sequence table does not contain LimsKField1 column, the LimsID editor column is locked.

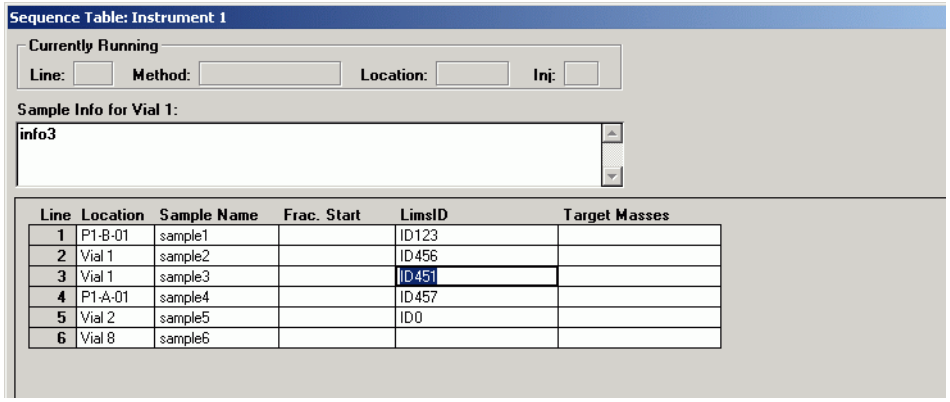

Figure 7 The Sequence Table columns

The new column is fully editable and allows changes to be made to the LimsKField1 of the sequence table itself. No error checking is provided; it is simply a string of maximum 40 chars length. It is the responsibility of the user to ensure that only logical values are stored.

Additional file in a raw datafile directory.

In Agilent ChemStation, the raw datafiles are not bound to the sequence table data; once the data has been acquired and analyzed, it has no direct relationship with the sample described as a row of the sequence table. The additional LimsKFields imported to the sequence table have to be stored along with the raw datafile, otherwise they will not be linked to the output data.

An additional XML file (limsinf.xml) is created in a raw datafile directory. The XML export uses the values to insert the LIMS information into the exported result file. The file has a very simple structure:

<?xml version="1.0" encoding="UTF-8"?>

<SampleLimsInfo xmlns:xsi="http:\\www.w3.org\2001\
XMLSchema-instance">

<LimsKField1>1</LimsKField1> (displayed as LimsID)

<LimsKField2>2</LimsKField2>

<LimsKField3>3</LimsKField3>

</SampleLimsInfo>

It contains the values of the sequence table's LimsKFieldN column for the corresponding sample.

The file is created at two hooks, only when a sequence is running and when the LIMS columns exist in the sequence table:

PostACQ (executed after DATA ACQUISITION)

PostDA (executed after DATA ANALYSIS)

The file can be overwritten when reprocessing the data. This is intentional: the user is allowed to change at least LimsKField1 value using the sequence table editor.

For the user, this means that after changing the LimsID in the sequence table, the sequence has to be reprocessed, so that the correct values get written into limsinf.xml.

The LIMS Fields Idea in Summary

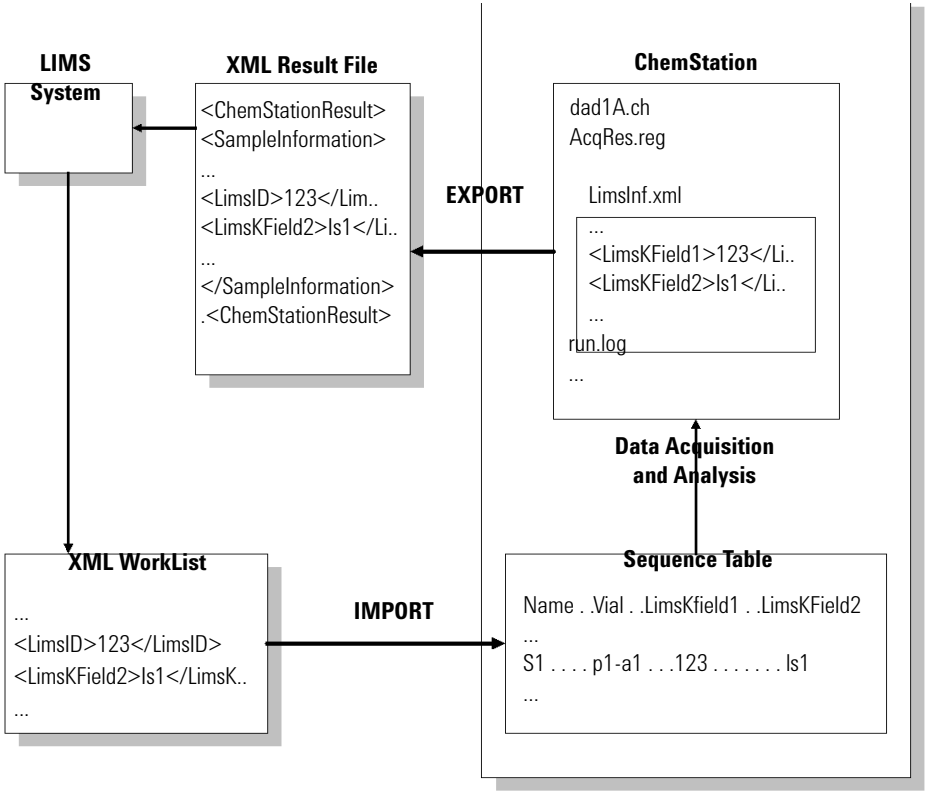

Figure 8 Persistence of the LIMS fields

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The XML-formatted result file is exported from the Agilent ChemStation and uploaded to the remote location if so configured. There are two modes:

- manual/interactive: a menu item and a button allow the user to export current results to an XML file and upload it to a remote directory
- automatic: the XML results file is generated automatically while a sequence is running and the file is copied to a remote directory if configured

The file is protected by a checksum, and the user has a possibility to check the integrity of the datafile with a command-line tool. If the first attempt at copying to the remote location fails, more attempts are made. If all attempts fail, the file is copied to the local directory.

General

The export process is driven by a macro that creates an XML file containing values taken from the CHROMREG and CHROMRES registers. The file is created either automatically (after the data analysis while the sequence is running) or manually (in Data Analysis view) using a button/menu item. The file is created in an appropriate raw datafile directory and copied to a remote location if *XMLAutomation*=1.

The report type is determined by the **Specify Report** settings of the method. The following settings affect the export file:

- Quantitative Results: results are always sorted by signal
- Style: Short, Detail, Header+Short, GLP+Short, GLP+Detail, Short+Spectrum, Detail+Spectrum, Full and Library Search all generate the same standard style of export file.
  Performance styles add an amount of complementary detail in accordance with the style name.
  None means that no quantitative Results section is included in the export file.
- Report Layout For Uncalibrated Peaks: Do Not Report means that no uncalibrated peaks are included in the Results section of the export file. The other options are treated identically: uncalibrated peaks are included.

Manual export

There is an additional menu entry in Data Analysis View, available only in Full Menu mode. It is present only when *XMLEnableExport*=1.

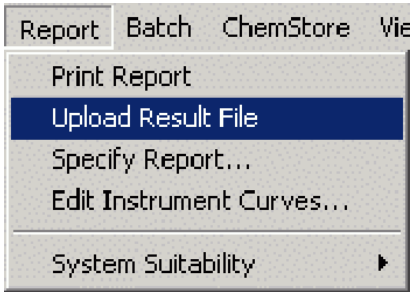

Figure 9 The Report menu for XML export

For the user's comfort, a tool is also available in the report section of the toolbar. It appears along with the other buttons of the section only when in Calibration Task or Integration Task mode. It also works in BATCH mode.

Figure 10 XML Batch tool

The actions are undertaken in three phases:

1 identify and calculate peaks.

If this is successful:

2 create the XML results file (result.xml) in the current raw datafile directory (the directory current data registers are loaded from).

If this is successful:

3 upload the file to the remote location.

Automatic export

The automatic export is done after data analysis for every sequence run, which means that if Data Analysis is not a part of the method, the file is not created.

The file (result.xml) is created in a current raw datafile directory and if *XMLAutomation*=1 it is uploaded to the remote directory in accordance with the settings in CHEMSTATION.INI. No user interface is necessary for automatic export.

The format of the XML results file.

The result file includes the following sections:

- Acquisition parameters
- Module information
- Sample information
- Chromatograms
- Results (Compound table)
- Custom results

Acquisition

Contains the version number of the acquisition software, instrument name and method modification data:

```
<Acquisition>
        <Version>Rev. A.02.02 Copyright (c) Hewlett Packard 1990-2003</Version>
        <InstrumentName>HP LC 1050</InstrumentName>
          ...
</Acquisition>
```

Module information

Contains a list of modules including: module name, serial number, firmware revision:

```
<ModuleInformation>
        <Module>
            <Number>1</Number>
            <NumberInModule>1</NumberInModule>
            <ModuleName>Analog/digital converter</ModuleName>
                ...
```

```
        </Module>
        <Module>
            <Number>2</Number>
                ...
        </Module>
        ...
</ModuleInformation>
```

Sample information

Contains software revision description, fields from a sequence table line belonging to the sample plus method path and description and injection date/time:

```
<SampleInformation>
        <Version>Rev. B.01.01 [xxxx] Copyright © Agilent Technologies</Version>
        <VialUnused>0</VialUnused>
        <SequencePath/>
        <Dilution>-1</Dilution>
        <InjVolume>2</InjVolume>
            ...
</SampleInformation>
```

Chromatograms

Grouped by signals:

```
<Chromatograms>
        <Signal>
            <Title>DAD1 A, Sig=254,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            <Description>DAD1 A, Sig=254,4 Ref=550,100</Description>
            ...
            <IntegrationResults>
                <RetTime Unit="min">0.74711</RetTime>
                <Area Unit="mAU*s">300.036407</Area>
                ...
            </IntegrationResults>
```

```
            <IntegrationResults>
            …
            </IntegrationResults>
        </Signal>
        <Signal>
            <Title>DAD1 B, Sig=230,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            …
        </Signal>
</Chromatograms>
```

Each SIGNAL group contains signal descriptions (i.e. title, detector, signal id, operator, X and Y Axis units etc.) and all integrated peaks of the signal (INTEGRATIONRESULTS) with a thorough description of each peak: RT, Area, Area%, Width.

If the “Performance+Noise” report style is used, the SIGNAL node contains also a group called NOISE, built of NOISEPERIOD subnodes. They hold all the noise data generated by “Performance+Noise” report style.

```
<Chromatograms>
        <Signal>
            <Title>DAD1 A, Sig=254,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            …
                <Noise>
               <NoisePeriod>
                <TimeFrom Unit="min">0</TimeFrom>
                <TimeTo Unit="min">0.5</TimeTo>
                <Noise6SD Unit="mAU">0.300586</Noise6SD>
                <NoisePToP Unit="mAU">0.192784</NoisePToP>
                <NoiseASTM Unit="mAU">0</NoiseASTM>
                <Wander Unit="mAU">0</Wander>
                <Drift Unit="mAU/h">16.720044</Drift>
               </NoisePeriod>
               <NoisePeriod>
               …
               </NoisePeriod>
            </Noise>
            <IntegrationResults>
            …
            </IntegrationResults>
```

```
            </Signal>
            ...
</Chromatograms>
```

Results

Contains the result of quantitative calculations, according to the current report settings. The two basic items describe:

- the type of calculation (Percent, ISTD,...)
- the base for calculation (Area, Height)

```
<Results>
    <QuantCalc>ESTD</QuantCalc>
    <QuantBase>Area</QuantBase>
    <ResultsGroup>
    ...
    </ResultsGroup>
    <ResultsGroup>
    ...
    </ResultsGroup>
 </Results>
```

The RESULTSGROUP nodes contain peak groups.

When the calculation is of a percent type, peaks are grouped by signals. The group description is a particular signal description then.

```
    <ResultsGroup>
        <ResultsGroupDescription>DAD1 A, Sig=254,4 Ref=550,100</ResultsGroup-
Description>
        <Peak>
        ...
        </Peak>
        <Peak>
        ...
        </Peak>
    </ResultsGroup>
    <ResultsGroup>
```

```
        <ResultsGroupDescription>DAD1 C, Sig=280,4 Ref=550,100</ResultsGroup-
Description>
        <Peak>
        …
        </Peak>
        <Peak>
        …
        </Peak>
    </ResultsGroup>
```

When the calculation is of any other type, there is only one group, called MAIN. It contains all the calculated peaks.

```
<ResultsGroup>
        <ResultsGroupDescription>MAIN</ResultsGroupDescription>
        <Peak>
        …
        </Peak>
        <Peak>
        …
        </Peak>
</ResultsGroup>
```

PEAK node represents a single peak/compound (in the “Percent” calculations all of the integrated peaks are the part of the result file, not only found compounds).

```
 <Peak>
        <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
        <PeakType>BB </PeakType>
        <ExpRetTime Unit="min">0.747087</ExpRetTime>
        <MeasRetTime Unit="min">0.74711</MeasRetTime>
        <Area Unit="mAU*s">300.036407</Area>
        <Height Unit="mAU">106.920616</Height>
        <Width Unit="min">0.044739</Width>
        <Symmetry>0.716419</Symmetry>
        <Name>Dimethylphthalate</Name>
        <Amount Unit="wt%">0.0905459542</Amount>
</Peak>
```

Apart from the basic data (the Signal it belongs to, Peak type, RT, Area, Height, ...), each peak contains the “amount” field which presents the result of the current quantitative calculations, and the name of the found compound (if the method supports calibration table with compound names).

In calculations of other type (not Percent) only compounds with the amount >0.0 are presented.

When a “Performance“-like results XML file is generated, additional nodes appear in a PEAK section:

```
<Peak>
    ...
    <kPrime>5.42268</kPrime>
    <PlatesHalfWidth>4080.07502</PlatesHalfWidth>
    <ResolutionHalfWidth>11.903108</ResolutionHalfWidth>
    <Selectivity>3.48661</Selectivity>
    <Skew>1.039269</Skew>
    <Excess>1.564137</Excess>
    ...
    and other performance results
</Peak>
```

When System Suitability -> Performance Limits are set the information about them appears as an attribute at the value affected by the limits.

A value is higher than the higher limit:

```
<kPrime Suitability=”>”>5.42268</kPrime>
```

A value is lower than the lower limit:

```
<PlatesHalfWidth Suitability=”<”>4080.07502</PlatesHalfWidth>
```

A value is between the limits:

```
<ResolutionHalfWidth Suitability=”=”>11.903108</ResolutionHalfWidth>
```

Custom results

Contains custom results from “XmlCustom” table.

Hooks and Custom Results Table

The XML results file supports custom results. This means that the exported file can contain the custom values structured in a simple tabular form.

Two additional hooks are available to the user:

XML_PreExport: executed just before the values from the CHROMREG/CHROMRES registers are exported.

XML_PostExport: executed after the XML results file has been created.

At the beginning of the export process, an empty *XmlCustom* table is created in the CHROMRES register. It contains two text columns (*Item* and *Text*) of maximum 255 characters:

XMLCUSTOM

Item	Text
...	...

Immediately after the table has been created, the *XML_PreExport* hook is triggered. It is intended to give the user an opportunity to fill the *XmlCustom* table with his/her own values.

Example of the macro:

Name *XML_FillCustomTableExample*

InsTabRow *ChromRes, "XmlCustom", 1:2*

SetTabText *ChromRes, "XmlCustom", 1, "Item", "ItemExample1"*

SetTabText *ChromRes, "XmlCustom", 1, "Text", "TextExample1"*

SetTabText *ChromRes, "XmlCustom", 2, "Item", "ItemExample2"*

SetTabText *ChromRes, "XmlCustom", 2, "Text", "TextExample2"*

EndMacro

A command:

SetHook *"XML_PreExport", " XML_FillCustomTableExample "*

sets the *XML_FillCustomTableExample* macro to be executed every time before exporting the file.

If the table is not empty, the following section are created as a part of the XML results file:

```
...
<CustomResults>
```

```
        <Info>
            <Item>ItemExample1</Item>
            <Text>TextExample1</Text>
        </Info>
        <Info>
            <Item>ItemExample2</Item>
            <Text>TextExample2</Text>
        </Info>
</CustomResults>
...
```

Having created the file, the exporting process executes the *XML_PostExport* hook and deletes the *XmlCustom* table.

Uploading the file: the copying process

The external application is responsible for copying an XML results file from the current raw datafile directory to a remote location. \Chem32\SYS\ Filecopy.exe is a 32-bit command line application that can operate on UNC paths as well as on local directories. It is used indirectly only by macros creating result files when the *XMLAutomation* variable exists and is equal to 1.

First, it tries to copy the file to the *XMLExportDestUNC$* directory. If this fails, the application sleeps for *XMLExportCopyWaitTime* seconds and tries again. The process is repeated *XMLExportCopyTries* times. If the copying is still unsuccessful, it copies the file to *XMLExportLocalRecovPath$* directory (if it exists).

The appropriate messages are logged in the Instrument's Log Book, informing about the result of copying process and sources of errors.

The name of the file

The name of the results file in the raw datafile directory is always the same: result.xml. The file is copied to the remote directory under a different name so as to:

1 make sure that the names are unique, since the files are copied to the same directory

2 make the names meaningful

The name is constructed as:

InstrumentName_SampleName_YYMMDDHHmmSS.xml

where the time included is the time of creating the file.

All the spaces in the instrument or sample's name are replaced with underscore "_"

Example:

HP_LC_1050_Isocratic_Std._1_030213111701.xml

NOTE

It is possible to use different naming convention for the name of the XML result file spooled to the remote directory. Two macros coming along on the ChemStation CD-ROM allow the user to choose between the following option:

LIMSID_DATE_TIME.xml or **DATE_TIME_LIMSID.xml**

Both solutions are based on macro usage. The installation and instructions to run the macros are documented in the readme.txt along with the macro. Macros and documentation can be found on the root directory of the *ChemStation CD-ROM, UCL, LC_UCL*. Please look at the index to identify the macro.

Checksums

The checksum for the XML file is calculated using the MD5 algorithm. The checksum is inserted into the file as a root node attribute:

<ChemStationResult checksum="ce117a6da2eaa3a91d92d6ba9699a0fb">

It is a hexadecimal form of 128 bits value, always containing 32 characters of [0-9a-f] range.

Just after the XML results file has been created, the line above contains the checksum attribute equal to: checksum=”00000000000000000000000000000000”. The external \Chem32\SYS\checksum.exe application calculates the 128 bits value for the file and then replaces the sequence of zeros with the calculated value.

The user is provided with the \Chem32\SYS\chkfile.exe command line tool to check the integrity of the XML results file. The tool extracts the checksum attribute from the XML file, replaces it temporarily with a sequence of zeros, calculates the checksum and compares it with the extracted one. If they are equal, it means that the XML file hasn’t been changed since it was created. The message is printed to the standard output of application.

6
XML in Agilent ChemStore

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Export-related entries 59
Import Worklist 60

This chapter explains how to use the previously described XML for Agilent ChemStation in conjunction with Agilent ChemStore. It shows how the workflow differs from ChemStation and the different Oracle tables & views that are used. As previously described in Chapter 1 XML is a very portable and flexible protocol for interconnectivity between systems.

NOTE Running XML using ChemStation Rev. A.10.x and ChemStore Rev. B.03.01 this manual is not applicable. Please refer to the appropriate XML Interface Guide in the manual section of your Rev. B.03.0x ChemStore CD-ROM.

Workflow using Agilent ChemStore

The workflow that describes the connectivity with ChemStore can be divided into five sequential activities shown in Figure 11:

1. The sample list is generated by the LIMS system in an XML format.
2. It is imported by Agilent ChemStation.
3. Samples are analysed, and spooled to ChemStore (automatically if Security Pack is installed).
4. Information typically required by LIMS systems are stored in two read-only views in the ChemStore ORACLE database.
5. If enabled on the system or a specific study , information goes through an Approval stage and is made available to an external LIMS system.
6. A program from the LIMS systems can scan a table in the ORACLE database to see if any new records are available for processing, and can amend the flag so that it not scanned subsequent scans.

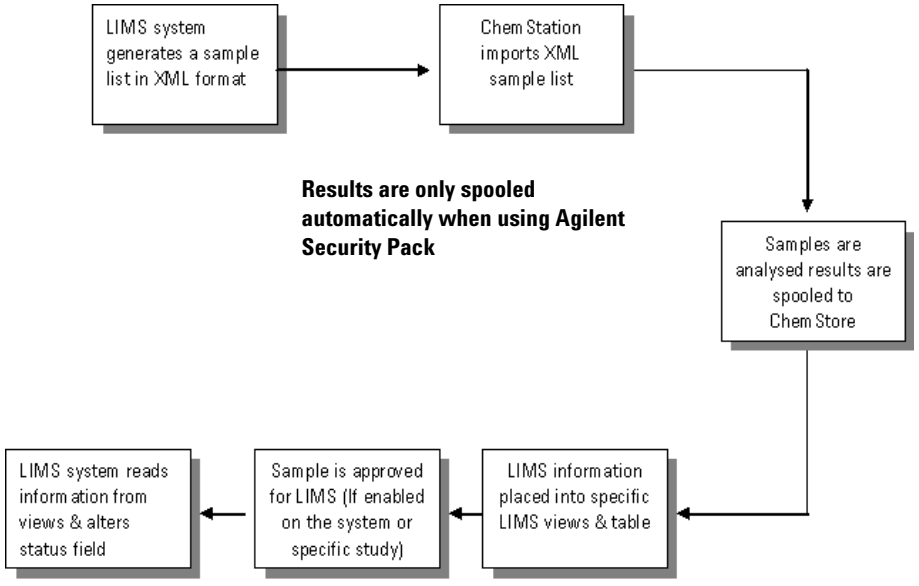
LIMS system generates a sample list in XML format
ChemStation imports XML sample list
Results are only spooled automatically when using Agilent Security Pack
Samples are analysed results are spooled to ChemStore
LIMS information placed into specific LIMS views & table
Sample is approved for LIMS (If enabled on the system or specific study)
LIMS system reads information from views & alters status field

Figure 11 Workflow using Agilent ChemStore

Results are only spooled automatically when using Agilent Security Pack.

The Agilent ChemStore XML interfaces has similarities to the ChemStation interface and uses the same scheme for the first two activities of the workflow:

- Import a worklist containing a sequence in XML format into ChemStation
- Data is spooled to ChemStore rather than creating an export back to LIMS
- (Ensure that the ChemStation.ini value for enabling export is set to value Zero)
- Data is read by the LIMS system from views & tables from within ChemStore
- The advantage of this scheme for ChemStore users is that the data is held in a secure environment with all the advantages of ChemStore, and only one export interface needs to be managed rather than multiple ChemStation interfaces.

Enabling XML Functionality for ChemStore

This section explains the changes that have to be made to enable the XML interface functions in the Agilent ChemStation to allow it to work with ChemStore.

The configuration is different to that of use with ChemStation interface.

XML functionality in the Agilent ChemStore is enabled by entries in the ChemStation-related sections of CHEMSTATION.ini file. Two entries in the [PCS] section of the CHEMSTATION.ini enable the complete XML export/import functionality although the export will be turned off as it utilises ChemStore functionality.

NOTE It is possible to export from ChemStation as well as ChemStore by enabling the functionality in the [PCS] section of CHEMSTATION.INI, but this information is not subject of the new features in ChemStore of Approval, Run Locking or the LIMS notification features.

[PCS]

XMLEnableImport=1

XMLEnableExport=0 (See note above)

The lack of the entry or entry=0 turns off the functionality.

Import-related entries

In the section for each instrument, [PCS,n], a variable specifies the default directory for importing files. This directory in which the import file dialog opens, and where the manual import function looks for a file with no specified path.

[PCS,n]

XMLImportPath$=d:\xml\xml

Export-related entries

As exporting of data is handled within ChemStore there are no required entries in the CHEMSTATION.INI file. It may be that legacy entries exist in CHEMSTATION.INI and it is recommended to read the appropriate section of the manual to see what they are.

Import Worklist

Three additional columns are available to be imported into ChemStation via the XML interface. These are:

- LIMS ID
- LimsKField2, and
- LimsKField3

All three values are string values with the maximum size of 40 characters. These values are transferred to ChemStore as custom fields.

For more information on this function see the ChemStation Import Worklist.

NOTE During the XML import it is only possible to view the column with the LIMS ID. The other LIMS fields (LimsKField, LimsKField3) are imported but not displayed within the import tool.

7
ChemStore for LIMS interfacing

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LIMS Notification configuration 66

This chapter describes the configuration of ChemStore to allow the export of runs to LIMS.

NOTE This feature was introduced in ChemStore revision B.03.01

General

The configuration of a LIMS export is managed globally per database or an individual study basis. There are three factors to consider when configuring the LIMS export Figure 12:

- Approval Configuration
- Run locking
- Lims notification

Configuration of these features is at two levels. They can be set either on a per system basis (see Figure 13 on page 63) or on an individual study basis (see Figure 15 on page 64). The system configuration serves as a template for newly created studies, where further modifications are done individually. The study configuration takes priority over the system configuration.

Configuration of these three features must be done according to individual work flows.

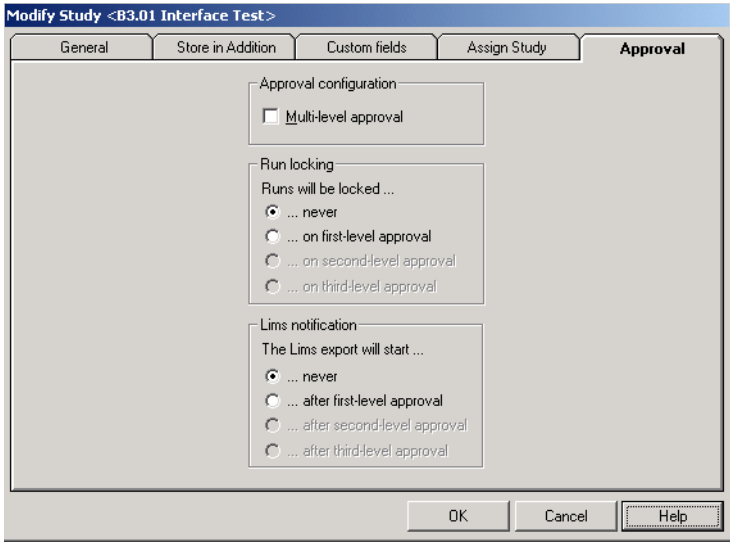

Figure 12 Individual Study Approval panel

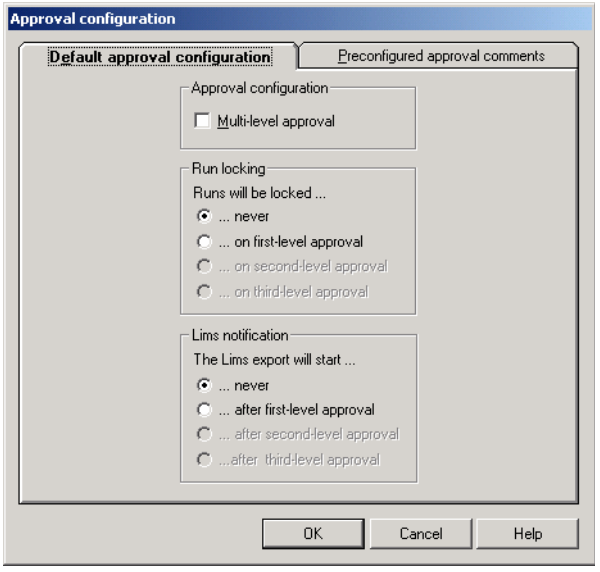

Figure 13 System template for default approval configuration

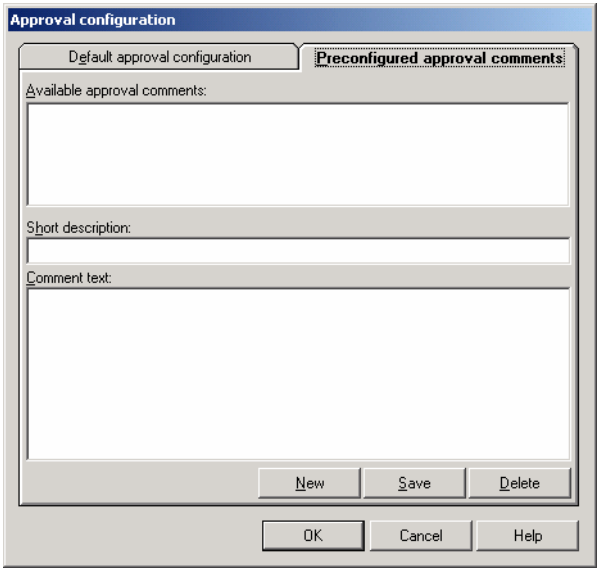

Figure 14 System preconfigured approval comments

It is possible to pre-configure a number of approval comments (See Figure 13 on page 63) which can be used when the approver approves a sample in ChemStore. If no comments are pre-configured then the approver will be prompted after each approval, these comments can only be configured globally (on a system basis).

Approval configuration

It is possible to define the usage of multiple approval levels on a per-study basis. The ability to approve runs and the level of approval are granted to an individual using the ChemStore account administration procedures, Figure 15:

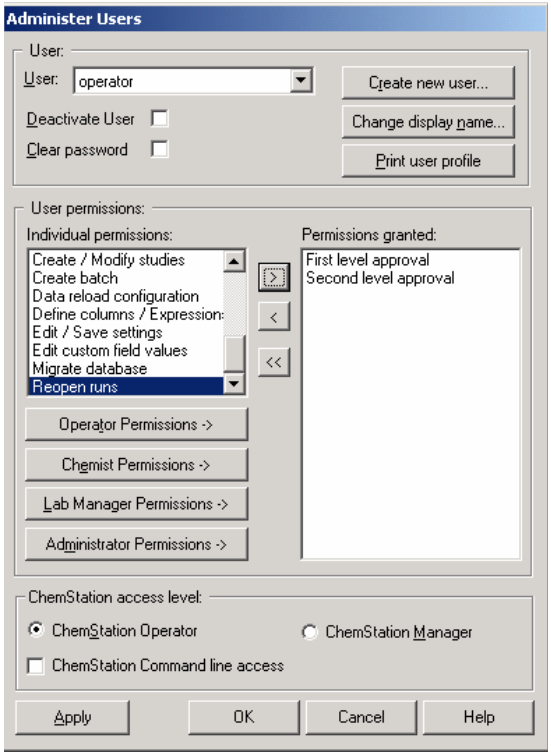

Figure 15 Granting approval permissions to an individual

Run Locking configuration

Approval of the results prior to 'Sample-locking' is critical as once this action is complete the results are fixed in the database and cannot be reloaded to ChemStation batch review for reprocessing (unless they were rejected again).

The options for this are as follows:

never

1 Choose the **never** option to specify that runs are never locked. This will retain the ability to review data in ChemStation batch review even after final approval.

on first-level approval

2 Choose the "**on first-level approval**" option to specify that runs are locked when first level approval is given.

on second-level approval

3 Choose the "**on second-level approval**" option to specify that runs are locked only when second level approval is given. This option is unavailable when the **Multi-level approval** check box is cleared.

on third-level approval

4 Choose the **„on third-level approval“** option to specify that runs are locked only when third level approval is given. This option is unavailable when the **Multi-level approval** check box is cleared.

LIMS Notification configuration

It is important that the result in LIMS matches the result in ChemStore and is updated when a change has occurred. Therefore the LIMS notification options should be configured to match the options selected in the approval configuration for approval and run locking as well as the laboratory workflow.

never

1 Choose the **never** option to specify that runs are never exported to LIMS.

after first-level approval

2 Choose the „**after first-level approval**“ option to specify that runs are exported after first level approval is given.

after second-level approval

3 Choose the „**after second-level approval**“ option to specify that runs are exported only after second level approval is given. This option is unavailable when the **Multi-level approval** check box is cleared.

after third-level approval

4 Choose the „**after third-level approval**“ option to specify that runs are exported only after third level approval is given. This option is unavailable when the **Multi-level approval** check box is cleared.

8 LIMS ORACLE Views and Tables within ChemStore and extacting their data

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ChemStore Query 75

This chapter describes the contents of Oracle views and tables used for storage of information which can be used by a LIMS system to extract the required data. Additionally, this chapter discusses possible ways of extracting the data from the ORACLE views and tables with a query in ChemStore.

Views and Tables

ChemStore samples are uniquely identified by a combination of the following items:

- the Injection ID (identifying an acquisition)
- the Study ID (identifying the study the data is stored in)
- LIMS ID (when specified)

NOTE The LIMS ID must be unique!

For convenience the combination of all three will be referred to as a 'sample'

Beginning with B.03.01 the Oracle database includes two new views and a table, which contain information typically used by LIMS systems. The information cover three area:

- **Sample Information** (including basic Sequence and Instrument information)
- **Run Information** (a reprocessing version is called a run) including Approval states
- **Peak Information**

Definitions

The new Views and Table are defined as follows:

Views

- **LIMS_SAMPLE:**
- Containing sample and run information along with LIMS specific fields
- **LIMS_RESULT:**
- Containing peak information (relation to LIMS_SAMPLE is 1:n)

Table

- **LIMS_Flag:**
- Containing sample and run information along with fields, which writeable by the LIMS system.

Content of the View LIMS_SAMPLE

Table 2 Content of the View LIMS_SAMPLE

Field Name	Field Type	Description
INJ_ID	Numeric	Injection ID
RNG_ID	Numeric	Study ID
LIMS_ID	Numeric	Custom field transferred from LIMS
LIMSKFIELD2	String	Custom field transferred from LIMS
LIMSKFIELD3	String	Custom field transferred from LIMS
STUDYNAME	String	Study Name
VERSION	Numeric	Run Version
APPROVALSTATE	String	LIMS Approval State
PROCESSEDBYLIMS	Numeric	Flag field used by LIMS interface via LIMS_FLAG table providing Acknowledgement mechanism. Processed by LIMS: 0 New injection spooled: 1 New run version spooled: 2 Run version deleted while archiving: 3 Run status changed to 'Not approved': 4 Run status changed to 'Rejected': 5 Run status changed to 'Approved': 6
LIMSFLAG1	String	Custom flag fields that might optionally be used by LIMS system for any king of flagging purpose (see LIMS_FLAG)
LIMSFLAG2	String	Custom flag fields that might optionally be used by LIMS system for any king of flagging purpose (see LIMS_FLAG)

Table 2 Content of the View LIMS_SAMPLE (continued)

Field Name	Field Type	Description
LIMSFLAG3	String	Custom flag fields that might optionally be used by LIMS system for any king of flagging purpose (see LIMS_FLAG)
SAMPLENAME	String	Sample Name
AMOUNT	Numeric	Sample Amount
DILUTIONFACTOR	Numeric	Sample Dilution Factor
MULTIPLIER	Numeric	Sample Multiplier
VIAL	Numeric	Sample Injection Vial Number
VOLUME	Numeric	Sample Injection Volume
UNITS	String	Sample Injection Volume Units
SEQUENCENAME	String	Sample Processing Sequence Name
SEQLINE	Numeric	Sample Processing Sequence Line Number
SEQREPNO	Numeric	Sample Processing Sequence Rep. Number
RAWDATASTORED	Numeric	Raw Data Stored Flag
RAWDATANAME	String	Raw Data Filename
RAWDATATIME	Date	Raw Data Date/Time (Injection Time)
INSTRUMENTNAME	String	Instrument Name
INSTRUMENTHOST	String	Instrument Host Name

Content of the View LIMS_RESULT

Table 3 Content of the View LIMS_RESULT

Field Name	Field Type	Description
INJ_ID	Numeric	Injection
RNG_ID	Numeric	Study
LIMS_ID	Numeric	LIMS ID

Table 3 Content of the View LIMS_RESULT (continued)

Field Name	Field Type	Description
CPDNAME	String	Compound (Peak) Name
RT	Numeric	Retention Time
CORRECTEDRT	Numeric	Corrected Expected Retention Time
AREA	Numeric	Area
AREAPERCENT	Numeric	Area %
HEIGHT	Numeric	Height
WIDTH	Numeric	Width
SYMMETRY	Numeric	Symmetry
AMOUNT	Numeric	Amount
ISTD	Numeric	ISTD Amount
QUALIFIED	Numeric	Qualified Flag
ASSIGNED	String	Assigned
BASELINE	Numeric	Baseline
CALIBPEAK	String	Calibration Peak
EXPMOBILITY	Numeric	Expected Mobility
MOBILITY	Numeric	Measured Mobility
SELECTIVITY	Numeric	Selectivity
SKEW	Numeric	Skew
MOMENT0	Numeric	Moment 0
MOMENT1	Numeric	Moment 1
MOMENT2	Numeric	Moment 2
MOMENT3	Numeric	Moment 3
MOMENT4	Numeric	Moment 4

Content of the Table LIMS_FLAG

Table 4 Content of the View LIMS_SAMPLE

Field Name	Field Type			Description
INJ_ID	NUMBER(10)	N/A	NO	Injection ID
RNG_ID	NUMBER(10)	N/A	NO	Study ID
LIMS_ID	VARCHAR(255)	N/A	YES	LIMS ID
RN_ID	NUMBER(10)	N/A	NO	Internal Run ID
LIMS_KFIELD2	VARCHAR(255)	N/A	YES	LIMS field
LIMS_KFIELD3	VARCHAR(255)	N/A	YES	LIMS field
LF_PF	NUMBER(1)	0	NO	Flag Field, used by LIMS system to identify Runs that were successfully processed by LIMS. Default value is 0 (not processed)
LF_CF1	VARCHAR(255)	NULL	YES	Custom flag field that might be used by LIMS system for any LIMS specific functionality
LF_CF2	VARCHAR(255)	NULL	YES	Custom flag field that might be used by LIMS system for any LIMS specific functionality
LF_CF3	VARCHAR(255)	NULL	YES	Custom flag field that might be used by LIMS system for any LIMS specific functionality

These views are updated automatically. This means they are filled as soon as a sample with a **LIMS ID** is transferred to ChemStore. When the sample is approved with the correct level of approval as specified in the approval configuration, the LIMS approval state will reflect this. As previously described, this function is configurable on a per study basis.

Oracle authentication & permissions

In order that a LIMS system can access the views and table the following ORACLE user credentials are required:

- Oracle User: LimsAccess

- Password: Password4Lims (initial password)

NOTE It is recommended that a suitably trained person change this password.

The user LimsAccess is granted the following permission or access to Oracle objects:

- Connect to Database (create session)
- Select from view LIMS_SAMPLE
- Select from view LIMS_RESULT
- Select from table LIMS_FLAG

The user can update the following fields in table LIMS_FLAG

- LF_PF
- LF_CF1
- LF_CF2
- LF_CF3

Extraction of information from Oracle Views

It is anticipated that each LIMS system and company will have different methods for extracting information on a regular frequency.

One possible way is to execute a program, which scans the LF_PF field in the LIMS_FLAG table on a regular basis to see if any new records are awaiting processing (any new entry will have the default value zero), once processed the value is altered so it is omitted from the next scan.

As the scan time for this table will vary depending on the number of records it is not recommended to submit the request on a time basis, for example every minute, but to use a program with a wait loop so that multiple requests are not trying to modify the same record.

It is also possible for the extracting program to add information to the additional three fields LF_CF1, LF_CF2, LF_CF3.

ChemStore Query

This section describes where the three LIMS fields can be found in the ChemStore database.

Once the information has been transferred from ChemStation it is possible to add the three new LIMS fields to your query selections as well as to the table columns in the user interface. (LIMS ID, LimsKField2, LIMSKField3).

These fields are available as **Custom Fields**, for example in the query builder as shown in Figure 16.

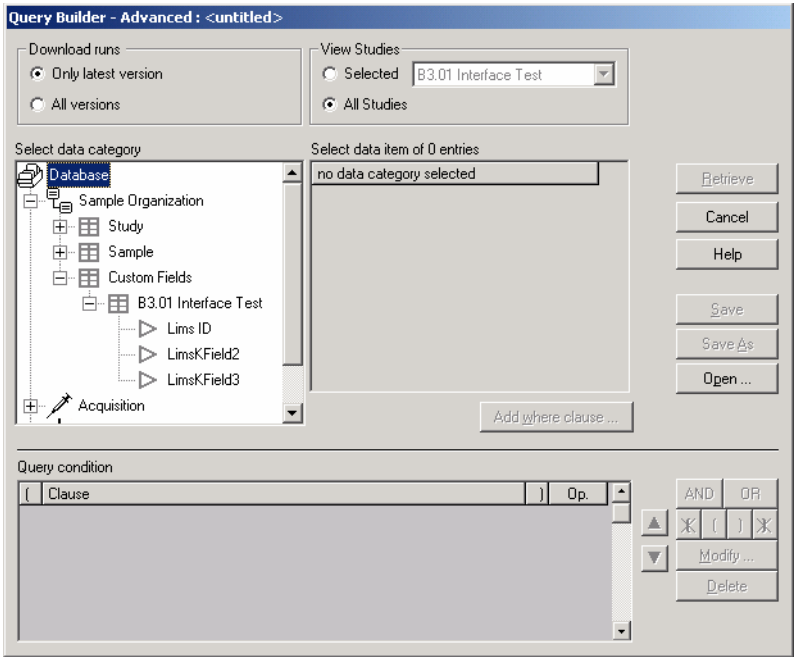

Figure 16 Custom Fields showing LIMS fields

9 Generic XML based Archive/Restore interface between ChemStore and an Archive or Data Management System (DMS)

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Restoring 82

This chapter defines the concept employed in creating a link between ChemStore and any Archive or Data Management System (DMS) for managing archives from a ChemStore client-server system for long-term storage. This concept employs the archival and restore of data by the use of the XML based **Archive/Restore** interface. Additionally it details the flow of data for restoration of information, this process which is currently an interactive process using both the DMS and the ChemStore application to ensure that files are correctly restored to their original location.

Overview

This section of the XML guide describes the XML features used in conjunction with the ChemStore Archiver. Based on XML files the ChemStore Archiver can be linked to external devices or systems. The primary purpose is to interface to Archive or Data Management Systems. But the same technology can be employed with media forms such as Tapes, DVD's or CD-ROM's.

The code required to develop the generic interface has already been shared with a number of the major archive management system vendors and they have already configured interfaces to their systems. An example is published as an Agilent application note with the publication number 5988-9912EN.

NOTE This feature has been available in ChemStore since revision B.02.02.

Background

At set of several hundred runs from ChemStore can, when archived, be stored in a single archive unit; an archive unit contains all versions of the specified runs. The archive unit is created either automatically or manually, as described in the ChemStore Concepts Guide. When setting up the archive unit the user can also add a description of the archive unit. However this description is generic and does not provide any details about the actual content of the archive unit. When ChemStore C/S creates the archive unit, it attaches a system-generated archive ID and a catalog file in XML format describing the contents of the binary archive unit down to the sample and result level. The file name corresponds to the name of the archive unit with the extension XML.

The generic XML archive interface has a design that introduces a layer between ChemStore and the DMS systems, based on XML. Custom plug-ins can be developed to interface the applications and further automate the archival of data. A so called '**Simple Plug-in**' is delivered with the interface. It serves as an example of a custom plug-in and provides an easy command line **Application Plug In**, for example to launch the Windows Messenger Service upon creation of a new archive. It does not require any further configuration.

The general concept of the interface can be seen in Figure 17.

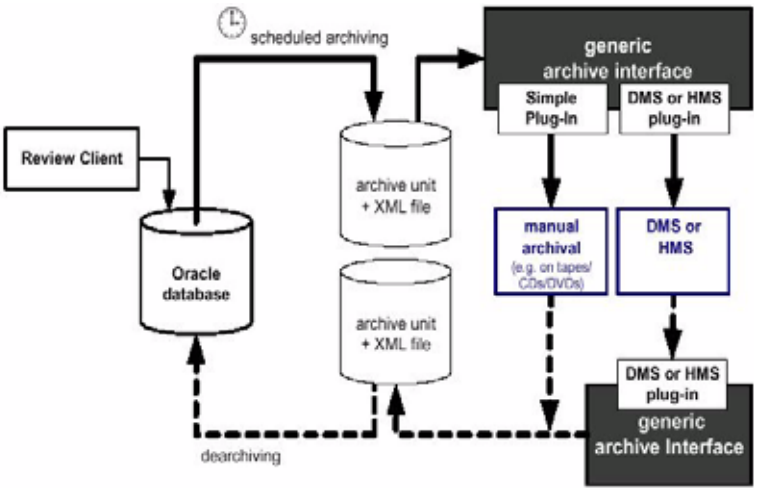

Figure 17 Generic XML-based archive interface

Although the diagram shows the archiving and restore procedure as two separate boxes they are actually just a single plug-in which serves both.

Installation of the configuration tool is performed on the same client as the archive is scheduled.

ChemStore Archiving

With ChemStore the built-in archiver will create an archive catalog in XML format for each archive unit containing detailed information on the content of the binary archive file.

When the XML-based Archive / Restore API is installed on the archiving client ChemStore will automatically communicate with the Generic XML based **Archive/Restore** interface to provide the information on the location of both files.

This then allows a transfer to begin to the DMS, this can be immediate or scheduled on a time basis. Once this has been completed the DMS can send a report back to the generic XML-based interface, which in turn notifies ChemStore that the transfer has been completed.

Restoring

Restoring an archive file can be done in two ways, initiated by ChemStore (when the archive file is known) and on the request of the DMS system (this is usually interactive as the user interactively defines multiple runs for review in ChemStore). The whole process is a manual operation with the DMS placing the binary archive file back to its original location, then ChemStore placing the information back into the database.

10
Installation & Configuration

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Configuration 85

The chapter details the installation and configuration of the XML-based **Archive/Restore** plug-in.

Installation

In order to use the XML **Archive/Restore** interface the software must be installed from the ChemStore CD. The Software is located in **<CD_Drive>:\G1410A\archiver_interface**.

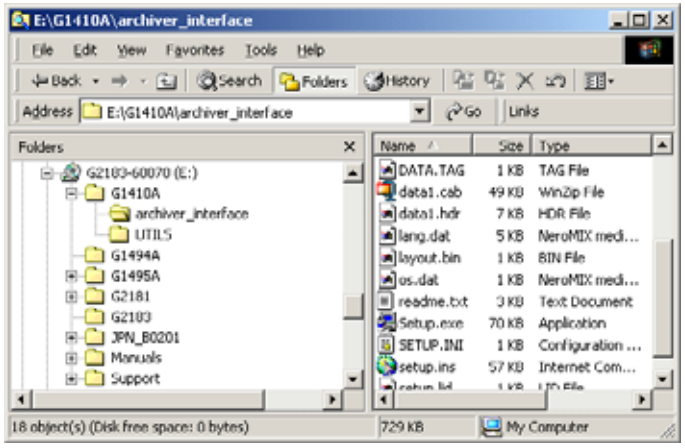


Figure 18 Installation of the Archive/Restore Interface software

Configuration

1 Install the software by executing the **setup.exe** file and follow the screen prompts.

NOTE It is possible to install the software from the run command prompt using the following command. <CD_Drive>:\G1410A\archiver_interface\setup.exe.

2 After installation the **Configuration** tool is installed in the same location as the ChemStore software. **Start > Programs > ChemStore**.

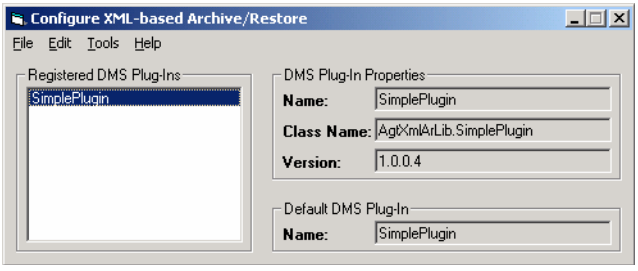


Figure 19 Configuration Tool for Archive/Restore Plug-in

A number of configuration options are available in the menu bar. This allows the addition or the removal of plug-ins as well as the changing of the properties. The default DMS Plug-in is **SimplePlugin** as shown in Figure 20.

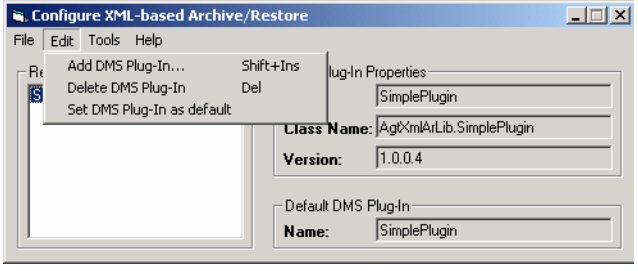


Figure 20 Plug-in options

The XML based **Archive/Restore** tools contains a number of options under the **Tools** menu item which assist in configuration and de-bugging of the configuration tool. Refer to Figure 21 and Figure 22.

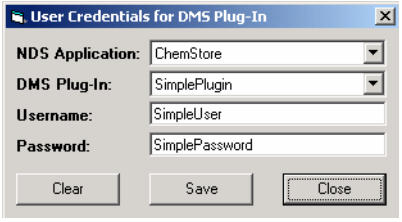


Figure 21 Setting application and user credentials

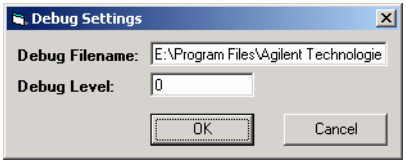


Figure 22 Setting the Debug File Location and Debug level

Additional information can be found in the online help of the tool.

By default the **Simple Plug In** triggers a dialog box popping up on the server PC each time a new archive file has been created, refer to Figure 23.

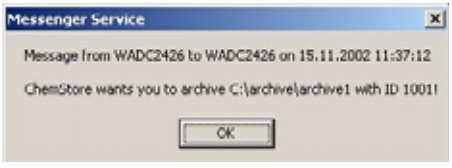
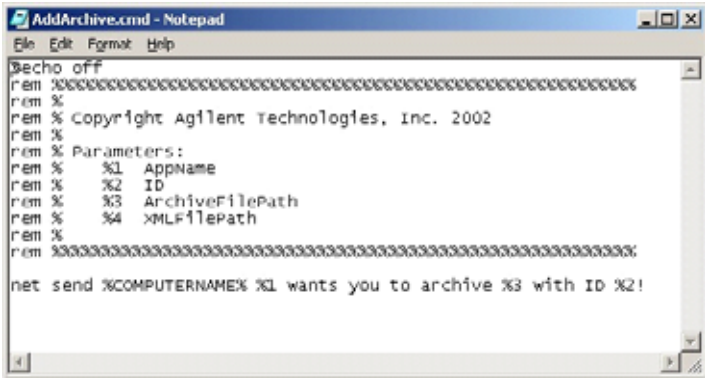

Messenger Service
Message from WADC2426 to WADC2426 on 15.11.2002 11:37:12
ChemStore wants you to archive C:\archive\archive1 with ID 10011
OK

Figure 23 Message created by the Simple Plug-in

The message and function of the **Simple Plug-in** can be changed by modifying the file **AddArchive.cmd** in the simple plug-in folder **"C:\Program Files\ Agilent Technologies\XML-based Archive Restore\Examples\Simple Plugin"**. The default content of the file is shown in Figure 24.


AddArchive.cmd - Notepad
File Edit Format Help
@echo off
rem %%%%

11
XML Schema Definition (XSD) for Archive Catalogue File

XML Schema Definition (XSD) for Archive Catalog File 90

This chapter describes the generic structure of the XML catalog file generated by the ChemStore.

NOTE This example is based on an example from ChemStore revision B.02.02

XML Schema Definition (XSD) for Archive Catalog File

Short Description of Main Nodes

The XML file can have only one root node with the tag **<ArchiveCatalog>**.

ArchiveCatalog node

The **<ArchiveCatalog>** node is the only root node and consists of one **<Head>** node, one **<Body>** node and an optional **<FileProtection>** node, in that order.

Head node

The **<Head>** node contains information describing the archive in detail, e.g. "Who started the archive", "When" and "On which PC?"

It contains nodes like **<Name>***, **<Description>**, **<Started>**, **<Computer>**, **<DirectoryPath>**, **<ArchiveSize>**, **<ProductName>**, etc. Most of the information is optional. For a detailed description see „detailed description“ and for an example XML file see the appendix I.

Body node

The **<Body>** node contains information describing the contents of the binary archive file. It consists of a number of **<User>** nodes, **<Instrument>** nodes, **<Method>** nodes, **<Project>**† nodes, **<Sequence>** nodes, and **<Sample>** nodes. Not all kinds of nodes have to be present, but they have to be in that particular order.

The information is organized in a sample-oriented way, because the main purpose of the XML file is to describe a binary archive file that will be stored in a sample-oriented Data Management System (DMS). Therefore, the nodes of most interest should be the **<Sample>** nodes. All other node types are only useful when starting from a **<Sample>** node.

*<Name> does not refer to the user who started the archive, but to the archive name, i.e. the archive filename.
†The <Project> node represents a ChemStore study. It is called Project for compatibility reasons.

If a **<FileProtection>** node is present, it consists of one **<HashValue>** node, containing a hash value that maintains the integrity of the file. Modifications to the XML file lead to an invalid hash value and can be recognized.

Sample node

The **<Body>** node contains a series of **<Sample>** nodes, one node for each injection, i.e. multiple **<Sample>** nodes are present if a sample has been injected multiple times. In addition, if an injection has been transferred to more than one study, a **<Sample>** node for each study will be present. A sample will contain two sub-nodes, an **<Acquisition>** node and a **<Result>** node.

Acquisition node

The **<Acquisition>** node contains all acquisition-specific data of an injection. A **<Sample>** node will always contain an **<Acquisition>** node, because ChemStore is a result-oriented database (ChemStation does only spool data to ChemStore after acquisition and data analysis have been completed).

Result node

The **<Result>** node contains the latest results generated by the data analysis of an injection, such as integration, calibration etc. Like all nodes, this node contains a Revision attribute. But unlike all the other nodes, the **<Result>** node's Revision attribute value is different from zero. It shows the number of times the data analysis has been run, a value of two or more means that the data have been reprocessed one ore more times and thus has two or more result versions. In this case the **<Result>** node's method could be different from the **<Acquisition>** node's method, etc.

Detailed Description

This section contains a non-declarative description of the XML Schema Definition version 1.02.03 (shipped with ChemStore C/S B.02.02 or higher). For the XML Schema Definition (XSD) file see appendix H.

Table 5 XML Schema definition

XML Path				Card.	Type	Example
<ArchiveCatalog>				1	[folder]	
	<Head>			1	[folder]	
		@ID		1	ID	1012
			<Name>	1	string	Testarchiv
			<Description>	1	string	Archiver test
		<Scheduled>		0..1	[folder]	
			<User> ...	1	UserRef	<ID>102</ID><Revision>0</Revision>
			<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
		<Started>		1	[folder]	
			<User> ...	1	UserRef	<Name/>
			<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
		<Completed>		1	[folder]	
			<User> ...	1	UserRef	<Name/>
			<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
			<Computer>	1	string	WADI1133
			<DirectoryPath>	1	string	C:\archive
			<ArchiveSize>	1	string	334741
			<ProductName>	1	string	ChemStore
			<ProductRevisionNumber>	1	string	B.02.02
			<DatabaseServerHostName>	1	string	WADI1133
			<ArchiveAndDelete>	1	boolean	true
<Body>				1	[folder]	
	<User>			0..n	[folder]	

Table 5 XML Schema definition (continued)

XML Path			Card.	Type	Example
	@ID		1	ID	102
	@Revision		1	uLong	0
	<Name>		1	string	admin
	<Description>		0..1	string	Administrator
	<Created>		0..1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Modified>		0..1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Status>		0..1	string	Active
<Instrument>			0..n	[folder]	
	@ID		1	ID	1001
	@Revision		1	uLong	0
	<Name>		1	string	HP LC 1050
	<Modified>		0..1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
<Method>			0..n	[folder]	
	@ID		1	ID	2130
	@Revision		1	uLong	0
	<Name>		1	string	BATCH.M
	<Description>		0..1	string	Method comment
	<Modified>		0..1	UserRef	
		<User> ...	1	UserRef	<Name/>

Table 5 XML Schema definition (continued)

XML Path			Card.	Type	Example
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Quantification Method>		0..1	string	ESTD
<Project>			0..n	[folder]	
	@ID		1	ID	1002
	@Revision		1	uLong	0
	<Name>		1	string	study
	<Description>		0..1	string	Test study
	<Created>		0..1	[folder]	
		<User> ...	1	UserRef	<ID>102</ID><Revision>0</Revision>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Modified>		0..1	[folder]	
		<User> ...	1	UserRef	<ID>102</ID><Revision>0</Revision>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Status>		0..1	string	Active
<Sequence>			0..n	[folder]	
	@ID		1	ID	1001
	@Revision		1	uLong	0
	<Name>		1	string	SEQUENCE.S
	<Description>		0..1	string	Example Sequence
	<Modified>		0..1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
<Sample>			0..n	[folder]	

Table 5 XML Schema definition (continued)

XML Path			Card.	Type	Example
	@ID		1	ID	1001
	@Revision		1	uLong	0
	<Name>		1	string	Isocratic Std. 1
	<Created>		0..1	[folder]	
		<User> ...	1	UserRef	<Name>a.g.h.</Name>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Type>		1	string	Calibration
	<BarCode>		0..1	string	<none>
	<CalibLevel>		0..1	uLong	1
<Acquisition>			0..1	[folder]	
		@ID	1	ID	2130
		@Revision	1	uLong	0
		<Name>	1	string	
	<Created>		0..1	[folder]	
		<User> ...	1	UserRef	<Name>a.g.h.</Name>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
	<Sequence> ... (Name only)		0..1	SeqRef	
		<Name>	1	string	SEQUENCE.S
	<Method> ... (Name+Time only)		0..1	MethRef	
		<Name>	1	string	DEMO.M
		<Modified>	0..1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00

Table 5 XML Schema definition (continued)

XML Path			Card.	Type	Example
	<Instrument> ...		0..1	InstRef	<ID>1001</ID><Revision >0</Revision>
	<RawData>		0..n	[folder]	
		@ID	1	uLong	2130
		@Revision	1	string	0
		<Name>	1	string	005-0101.D
		<Description>	0..1	string	this is a nice file
	<Created>		1	[folder]	
		<User> ...	1	UserRef	<Name/>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
		<Computer>	0..1	string	CSCLIENT00
		<DirectoryPath>	0..1	string	C:\CHEM32\2\DATA\ DEMO\
	<Signals>		0..1	[folder]	
	<Channel>		0..n	[folder]	
		<Name>	1	string	DAD1 A, Sig=254,4 Ref=550,100
		<Type>	1	string	Absorbance
			0..n	[folder]	
	@ID		1	ID	2296
	@Revision		1	uLong	2
	<Name>		1	string	
<Created>			0..1	[folder]	
		<User> ...	1	UserRef	<ID>102</ID><Revision> 0</Revision>
		<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00

Table 5 XML Schema definition (continued)

XML Path				Card.	Type	Example
	<Sequence> ...			0..1	SeqRef	<Name/>
	<Project> ...			0..1	ProjRef	<ID>1002</ID><Revision >0</Revision>
	<Method> ...			0..1	MethRef	<ID>2130</ID><Revision >0</Revision>
	<Compounds>			0..1	[folder]	
		<Compound>		0..n	[folder]	
			<Name>	1	string	Dimethylphthalate
			<RT>	1	double	0.746753454208374
			<Corrected RT>	1	double	0.747020646929741
			<Height>	1	double	104.845626831055
			<Area>	1	double	294.609161376953
			<Amount>	1	double	54.4980227705477
			<RF>	1	double	0.184984141415811
	<CustomFields>			0..1	[folder]	
			<CustomField>	0..n	[folder]	
			<Name>	1	string	test_custom_field
			<Value>	1	string	Test 1
			@Type	0..1	string	string
			<Unit>	0..1	string	mg
	<Approval>			0..1	[folder]	
		<User> ...		1	UserRef	<ID>102</ID><Revision> 0</Revision>
			<DateTime>	1	dateTime	2002-12-31T23:59:59+1:00
			<Description>	0..1	string	ArID: 1012
			<Status>	1	string	Approved

Table 5 XML Schema definition (continued)

XML Path	Card.	Type	Example
<FileProtection>	0..1	[folder]	
<HashValue>	1	string	UmgFiiCWbXQQdBWpZwJ2J88Y

XML Path

<bold_XML_tag>	complex XML tag, i.e. contains nested XML tags (e.g. <Sample>)
<XML_tag>	simple XML tag (e.g. <Name>)
@XML_attribute	XML Attribute (e.g. <Value Type=real>1.75</Value>)

Cardinality

1	Item required
0..1	Item optional
0..n	0, 1, 2 or an infinite number of items

Type

String	Any string (e.g. „Sample Name“)
Double	Any real number (e.g. 5.67)
Ulong	Any unsigned number (0, 1,...)
Boolean	boolean value (1, 0, true or false)
DateTime	Date and time (e.g. 2002-12-31T23:59:59+1:00)
ID	an object ID string (e.g. 1001)
XxxRef	either an object reference using <ID> and <Revision> or simply <Name>
[folder]	see <bold_XML_tag>

Example:

Blue background	constant value for all objects
Yellow background	see <bold_XML_tag>

A
Example Result File

This appendix contains an example of a results file that includes extended results.

```
<?xml version = "1.0" encoding="ISO-8859-1"?>
 <ChemStationResult xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="C:\Chem32\CORE\export.xsd" check-
sum="d50fb25d668361554903d6bb6a88f600">
  <Acquisition>
   <Version>Rev. A.02.02 Copyright (c) Hewlett Packard 1990-1993</Version>
   <InstrumentName>HP LC 1050</InstrumentName>
   <MethodPath/>
   <InjectionTime>1:00:00 AM</InjectionTime>
   <MethodLastModifiedTime>1:00:00 AM</MethodLastModifiedTime>
   <MethodLastModifiedBy/>
   <MethodModifiedAtRun>0</MethodModifiedAtRun>
  </Acquisition>
  <ModuleInformation>
   <Module>
    <Number>1</Number>
    <NumberInModule>1</NumberInModule>
    <ModuleName>Analog/digital converter</ModuleName>
    <SerialNumber/>
    <FirmwareRevision>Rev C.01.00</FirmwareRevision>
   </Module>
   <Module>
    <Number>2</Number>
    <NumberInModule>1</NumberInModule>
    <ModuleName>Pump</ModuleName>
    <SerialNumber/>
    <FirmwareRevision>3.1</FirmwareRevision>
```

```
  </Module>
  <Module>
    <Number>3</Number>
    <NumberInModule>1</NumberInModule>
    <ModuleName>Autosampler</ModuleName>
    <SerialNumber/>
    <FirmwareRevision>4.0</FirmwareRevision>
  </Module>
  <Module>
    <Number>4</Number>
    <NumberInModule>1</NumberInModule>
    <ModuleName>Diode array detector</ModuleName>
    <SerialNumber/>
    <FirmwareRevision>1.0</FirmwareRevision>
  </Module>
</ModuleInformation>
<SampleInformation>
  <Version>Rev. B.01.01 [xxxx] Copyright © Agilent Technologies</Version>
  <VialUnused>0</VialUnused>
  <SequencePath/>
  <Dilution>-1</Dilution>
  <InjVolume>2</InjVolume>
  <ActInjVolume>2</ActInjVolume>
  <AcqInstName>HP LC 1050</AcqInstName>
  <SeqLine>1</SeqLine>
  <Location>Vial 5</Location>
  <Inj>2</Inj>
  <Method>DEMO.M</Method>
  <Operator>a.g.h.</Operator>
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</SampleInformation>
<Chromatograms>
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 <SignalId>A</SignalId>
 <Operator>a.g.h.</Operator>
 <DateTime>4/19/94 7:52:24 AM</DateTime>
 <DerivOrder>0</DerivOrder>
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 <End>6.962083</End>
 <XUnits>min</XUnits>
 <YUnits>mAU</YUnits>
 <IntegrationResults>
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  <AreaPercent Unit="%">29.85427</AreaPercent>
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  <Height Unit="mAU">106.920616</Height>
  <HeightPercent Unit="%">46.40455</HeightPercent>
  <HeightSum Unit="mAU">230.409767</HeightSum>
  <Width Unit="min">0.044739</Width>
  <Symmetry>0.716419</Symmetry>
  <Baseline>0.039978</Baseline>
  <TimeStart Unit="min">0.695417</TimeStart>
  <LevelStart>0.230399</LevelStart>
  <BaselineStart>0.027093</BaselineStart>
  <TimeEnd Unit="min">0.922083</TimeEnd>
  <LevelEnd>0.24495</LevelEnd>
  <BaselineEnd>0.083591</BaselineEnd>
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  <Area Unit="mAU*s">275.973206</Area>
  <AreaPercent Unit="%">27.45993</AreaPercent>
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  <Height Unit="mAU">79.915726</Height>
  <HeightPercent Unit="%">34.684175</HeightPercent>
  <HeightSum Unit="mAU">230.409767</HeightSum>
  <Width Unit="min">0.052289</Width>
  <Symmetry>0.699074</Symmetry>
```

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  <Baseline>0.108524</Baseline>
  <TimeStart Unit="min">0.96202</TimeStart>
  <LevelStart>0.550645</LevelStart>
  <BaselineStart>0.093545</BaselineStart>
  <TimeEnd Unit="min">1.18875</TimeEnd>
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  <AreaPercent Unit="%">17.588933</AreaPercent>
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  <Height Unit="mAU">26.735945</Height>
  <HeightPercent Unit="%">11.603651</HeightPercent>
  <HeightSum Unit="mAU">230.409767</HeightSum>
  <Width Unit="min">0.101136</Width>
  <Symmetry>0.62962</Symmetry>
  <Baseline>-0.038655</Baseline>
  <TimeStart Unit="min">2.455417</TimeStart>
  <LevelStart>0.13536</LevelStart>
  <BaselineStart>-0.036177</BaselineStart>
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  <LevelEnd>0.077134</LevelEnd>
  <BaselineEnd>-0.045186</BaselineEnd>
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  <AreaPercent Unit="%">25.096867</AreaPercent>
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  <Symmetry>0.669291</Symmetry>
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   <Description>DAD1 B, Sig=230,4 Ref=550,100</Description>
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   <Operator>a.g.h.</Operator>
   <DateTime>4/19/94 7:52:24 AM</DateTime>
   <DerivOrder>0</DerivOrder>
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   <End>6.962083</End>
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    <AreaPercent Unit="%">36.775681</AreaPercent>
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    <Height Unit="mAU">301.804749</Height>
    <HeightPercent Unit="%">53.555611</HeightPercent>
    <HeightSum Unit="mAU">563.535254</HeightSum>
    <Width Unit="min">0.036068</Width>
    <Symmetry>0.919298</Symmetry>
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    <TimeStart Unit="min">0.698083</TimeStart>
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    <LevelEnd>-42.619328</LevelEnd>
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    <AreaPercent Unit="%">34.241827</AreaPercent>
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  <HeightPercent Unit="%">39.603011</HeightPercent>
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  <TimeEnd Unit="min">1.464386</TimeEnd>
  <LevelEnd>-36.989391</LevelEnd>
  <BaselineEnd>37.279369</BaselineEnd>
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  <LevelStart>0.103844</LevelStart>
  <BaselineStart>0.074115</BaselineStart>
  <TimeEnd Unit="min">2.802083</TimeEnd>
  <LevelEnd>0.115898</LevelEnd>
  <BaselineEnd>0.039075</BaselineEnd>
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  <Area Unit="mAU*s">464.298767</Area>
  <AreaPercent Unit="%">26.143104</AreaPercent>
  <AreaSum Unit="mAU*s">1775.989422</AreaSum>
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  <HeightPercent Unit="%">5.488433</HeightPercent>
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  <Symmetry>0.66407</Symmetry>
  <Baseline>0.116811</Baseline>
```

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    <LevelEnd>0.157922</LevelEnd>
    <BaselineEnd>0.167281</BaselineEnd>
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  <Description>DAD1 C, Sig=280,4 Ref=550,100</Description>
  <Detector>DAD1</Detector>
  <SignalId>C</SignalId>
  <Operator>a.g.h.</Operator>
  <DateTime>4/19/94 7:52:24 AM</DateTime>
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  <End>6.962083</End>
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    <HeightSum Unit="mAU">112.066494</HeightSum>
    <Width Unit="min">0.044559</Width>
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    <Baseline>0.107379</Baseline>
    <TimeStart Unit="min">0.695417</TimeStart>
    <LevelStart>0.166858</LevelStart>
    <BaselineStart>0.105893</BaselineStart>
    <TimeEnd Unit="min">0.882083</TimeEnd>
    <LevelEnd>0.222046</LevelEnd>
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  <IntegrationResults>
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  <HeightPercent Unit="%">5.050921</HeightPercent>
  <HeightSum Unit="mAU">112.066494</HeightSum>
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  <Baseline>0.013593</Baseline>
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    <TimeEnd Unit="min">6.242084</TimeEnd>
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   <MeasRetTime Unit="min">0.74711</MeasRetTime>
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   <Height Unit="mAU">106.920616</Height>
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   <kPrime>0.867774</kPrime>
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   <Selectivity/>
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   <Excess>3.487737</Excess>
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   <WidthTailing>0.106667</WidthTailing>
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  <StatisticalMoment2>0.000491</StatisticalMoment2>
  <StatisticalMoment3>0.000013</StatisticalMoment3>
  <StatisticalMoment4>1.566e-006</StatisticalMoment4>
  <PlatesTangent>1552.502327</PlatesTangent>
  <Plates5Sigma>1174.085003</Plates5Sigma>
  <PlatesStatistical>1153.031523</PlatesStatistical>
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  <Selectivity>1.792272</Selectivity>
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  <Excess>1.360217</Excess>
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  <USPTailing>1.206689</USPTailing>
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  <StatisticalMoment1>1.029706</StatisticalMoment1>
  <StatisticalMoment2>0.000668</StatisticalMoment2>
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```
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  <Plates5Sigma>1504.323467</Plates5Sigma>
  <PlatesStatistical>1587.931583</PlatesStatistical>
  <ResolutionTangent>3.327396</ResolutionTangent>
  <Resolution5Sigma>2.855306</Resolution5Sigma>
  <ResolutionStatistical>2.885621</ResolutionStatistical>
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 <Peak>
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  <Height Unit="mAU">26.735945</Height>
  <Width Unit="min">0.101136</Width>
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  <Skew>1.039269</Skew>
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  <WidthTailing>0.26</WidthTailing>
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  <StatisticalMoment1>2.588773</StatisticalMoment1>
  <StatisticalMoment2>0.002983</StatisticalMoment2>
  <StatisticalMoment3>0.000169</StatisticalMoment3>
  <StatisticalMoment4>0.000041</StatisticalMoment4>
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  <Plates5Sigma>2320.358549</Plates5Sigma>
  <PlatesStatistical>2246.776872</PlatesStatistical>
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```

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    <ResolutionStatistical>9.689001</ResolutionStatistical>
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   <Peak>
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    <PeakType>BB  </PeakType>
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    <MeasRetTime Unit="min">5.849135</MeasRetTime>
    <Area Unit="mAU*s">252.22435</Area>
    <Height Unit="mAU">16.837481</Height>
    <Width Unit="min">0.222766</Width>
    <Symmetry>0.669291</Symmetry>
    <Name>o-Terphenyl</Name>
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    <kPrime>13.622837</kPrime>
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    <Selectivity>2.512196</Selectivity>
    <Skew>0.870258</Skew>
    <Excess>1.019275</Excess>
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    <WidthTailing>0.592</WidthTailing>
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    <PlatesStatistical>2543.872414</PlatesStatistical>
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    <Resolution5Sigma>9.37518</Resolution5Sigma>
    <ResolutionStatistical>9.631284</ResolutionStatistical>
   </Peak>
  </ResultsGroup>
</Results>
```

```
  <CustomResults>
  </CustomResults>
</ChemStationResult>
```

A Example Result File

B
Export File Schema (EXPORT.XSD)

This appendix lists the schema that is used to produce the results file for export.

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<?xml version="1.0" encoding="ISO-8859-1"?>
<!-- edited with XMLSPY v5 rel. 4 U (http://www.xmlspy.com) by Reiner Lange (Agilent Technologies) -->
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" elementFormDefault="qualified" attributeFormDefault="unqualified">
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        <xs:complexType>
            <xs:sequence>
                <xs:element name="Acquisition">
                    <xs:complexType mixed="true">
                        <xs:complexContent mixed="true">
                            <xs:extension base="AcquisitionType"/>
                        </xs:complexContent>
                    </xs:complexType>
                </xs:element>
                <xs:element name="ModuleInformation">
                    <xs:complexType mixed="true">
                        <xs:sequence>
                            <xs:element name="Module" minOccurs="0" maxOccurs="unbounded">
                                <xs:complexType mixed="true">
                                    <xs:complexContent mixed="true">
                                        <xs:extension base="ModuleType"/>
                                    </xs:complexContent>
                                </xs:complexType>
                            </xs:element>
                        </xs:sequence>
```

```
            </xs:complexType>
        </xs:element>
        <xs:element name="SampleInformation">
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                <xs:complexContent mixed="true">
                    <xs:extension base="SampleInformationType"/>
                </xs:complexContent>
            </xs:complexType>
        </xs:element>
        <xs:element name="Chromatograms">
            <xs:complexType mixed="true">
                <xs:sequence>
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                            <xs:complexContent mixed="true">
                                <xs:extension base="SignalType"/>
                            </xs:complexContent>
                        </xs:complexType>
                    </xs:element>
                </xs:sequence>
            </xs:complexType>
        </xs:element>
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        <xs:element name="CustomResults">
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                    curs="unbounded">
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                            <xs:complexContent mixed="true">
                                <xs:extension base="InfoType"/>
                            </xs:complexContent>
                        </xs:complexType>
                    </xs:element>
                </xs:sequence>
            </xs:complexType>
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    </xs:sequence>
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</xs:complexType>
```

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        <xs:element name="InstrumentName"/>
        <xs:element name="MethodPath"/>
        <xs:element name="InjectionTime"/>
        <xs:element name="MethodLastModifiedTime"/>
        <xs:element name="MethodLastModifiedBy"/>
        <xs:element name="MethodModifiedAtRun"/>
    </xs:sequence>
</xs:complexType>
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    <xs:sequence>
        <xs:element name="RetTime" type="Value"/>
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        <xs:element name="AreaPercent" type="Value"/>
        <xs:element name="AreaSum" type="Value"/>
        <xs:element name="Height" type="Value"/>
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        <xs:element name="HeightSum" type="Value"/>
        <xs:element name="Width" type="Value"/>
        <xs:element name="Symmetry" type="Value"/>
        <xs:element name="Baseline" type="Value"/>
        <xs:element name="TimeStart" type="Value"/>
        <xs:element name="LevelStart" type="Value"/>
        <xs:element name="BaselineStart" type="Value"/>
        <xs:element name="TimeEnd" type="Value"/>
        <xs:element name="LevelEnd" type="Value"/>
        <xs:element name="BaselineEnd" type="Value"/>
    </xs:sequence>
</xs:complexType>
<xs:complexType name="SampleInformationType">
    <xs:sequence>
        <xs:element name="Version"/>
        <xs:element name="VialUnused"/>
        <xs:element name="SequencePath"/>
        <xs:element name="Dilution"/>
        <xs:element name="InjVolume"/>
        <xs:element name="ActInjVolume"/>
        <xs:element name="AcqInstName"/>
```

```
            <xs:element name="SeqLine"/>
            <xs:element name="Location"/>
            <xs:element name="Inj"/>
            <xs:element name="Method"/>
            <xs:element name="Operator"/>
            <xs:element name="InjectionDateTime"/>
            <xs:element name="SampleName"/>
            <xs:element name="SampleInfo"/>
            <xs:element name="IstdNum"/>
            <xs:element name="InternalStandardAmount"/>
            <xs:element name="SampleAmount"/>
            <xs:element name="Multiplier"/>
            <xs:element name="MethodInfo"/>
            <xs:element name="CalMethod"/>
            <xs:element name="ResModDateTime"/>
            <xs:element name="LimsID" minOccurs="0"/>
            <xs:element name="LimsKField2" minOccurs="0"/>
            <xs:element name="LimsKField3" minOccurs="0"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="ModuleType">
        <xs:sequence>
            <xs:element name="Number"/>
            <xs:element name="NumberInModule"/>
            <xs:element name="ModuleName"/>
            <xs:element name="SerialNumber"/>
            <xs:element name="FirmwareRevision"/>
            <xs:element name="BuildNumber" minOccurs="0"/>
            <xs:element name="PartNumber" minOccurs="0"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="SignalType">
        <xs:sequence>
            <xs:element name="Title"/>
            <xs:element name="Description"/>
            <xs:element name="Detector"/>
            <xs:element name="SignalId"/>
            <xs:element name="Operator"/>
            <xs:element name="DateTime"/>
            <xs:element name="DerivOrder"/>
            <xs:element name="RawdataFile"/>
```

```
                <xs:element name="Start"/>
                <xs:element name="End"/>
                <xs:element name="XUnits"/>
                <xs:element name="YUnits"/>
                <xs:element name="Noise" minOccurs="0">
                    <xs:complexType>
                        <xs:sequence maxOccurs="unbounded">
                            <xs:element name="NoisePeriod" minOccurs="0">
                                <xs:complexType>
                                    <xs:sequence>
                                        <xs:element name="TimeFrom" type="Value"/>
                                        <xs:element name="TimeTo" type="Value"/>
                                        <xs:element name="Noise6SD" type="Value"/>
                                        <xs:element name="NoisePToP" type="Value"/>
                                        <xs:element name="NoiseASTM" type="Value"/>
                                        <xs:element name="Wander" type="Value"/>
                                        <xs:element name="Drift" type="Value"/>
                                    </xs:sequence>
                                </xs:complexType>
                            </xs:element>
                        </xs:sequence>
                    </xs:complexType>
                </xs:element>
                <xs:element name="IntegrationResults" type="IntegrationResultsType"
minOccurs="0" maxOccurs="unbounded"/>
            </xs:sequence>
        </xs:complexType>
        <xs:complexType name="CompoundType">
            <xs:sequence>
                <xs:element name="SignalDesc"/>
                <xs:element name="PeakType" type="Value"/>
                <xs:element name="ExpRetTime" type="Value"/>
                <xs:element name="MeasRetTime" type="Value"/>
                <xs:element name="Area" type="Value"/>
                <xs:element name="Height" type="Value"/>
                <xs:element name="Width" type="Value"/>
                <xs:element name="Symmetry" type="Value"/>
                <xs:element name="Name"/>
                <xs:element name="Amount" type="Value"/>
                <xs:sequence minOccurs="0">
                    <xs:element name="kPrime" type="Value"/>
```

```
                    <xs:element name="PlatesHalfWidth" type="Value"/>
                    <xs:element name="ResolutionHalfWidth" type="Value"/>
                    <xs:element name="Selectivity" type="Value"/>
                    <xs:element name="SignalNoiseRatio" type="Value" minOc-
curs="0"/>
                    <xs:sequence minOccurs="0">
                        <xs:element name="Skew" type="Value"/>
                        <xs:element name="Excess" type="Value"/>
                        <xs:element name="WidthHalfHeight" type="Value"/>
                        <xs:element name="Width5Sigma" type="Value"/>
                        <xs:element name="WidthTangent" type="Value"/>
                        <xs:element name="WidthTailing" type="Value"/>
                        <xs:element name="USPTailing" type="Value"/>
                        <xs:element name="TimeIncrement" type="Value"/>
                        <xs:element name="DataPoints" type="Value"/>
                        <xs:element name="StatisticalMoment0" type="Value"/>
                        <xs:element name="StatisticalMoment1" type="Value"/>
                        <xs:element name="StatisticalMoment2" type="Value"/>
                        <xs:element name="StatisticalMoment3" type="Value"/>
                        <xs:element name="StatisticalMoment4" type="Value"/>
                        <xs:element name="PlatesTangent" type="Value"/>
                        <xs:element name="Plates5Sigma" type="Value"/>
                        <xs:element name="PlatesStatistical" type="Value"/>
                        <xs:element name="ResolutionTangent" type="Value"/>
                        <xs:element name="Resolution5Sigma" type="Value"/>
                        <xs:element name="ResolutionStatistical" type="Value"/>
                    </xs:sequence>
                </xs:sequence>
            </xs:sequence>
        </xs:complexType>
        <xs:complexType name="CustomResultsType">
            <xs:sequence>
                <xs:element name="Info" type="InfoType" minOccurs="0" maxOc-
curs="unbounded"/>
            </xs:sequence>
        </xs:complexType>
        <xs:complexType name="InfoType">
            <xs:sequence>
                <xs:element name="Item"/>
                <xs:element name="Text"/>
            </xs:sequence>
```

```
    </xs:complexType>
    <xs:complexType name="ResultsType" mixed="true">
        <xs:sequence>
            <xs:element name="QuantCalc" type="xs:string"/>
            <xs:element name="QuantBase" type="xs:string"/>
            <xs:element name="ResultsGroup" minOccurs="0" maxOc-
curs="unbounded">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="ResultsGroupDescription"/>
                        <xs:element name="Peak" type="CompoundType" minOc-
curs="0" maxOccurs="unbounded"/>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="Value" mixed="true">
        <xs:attribute name="Unit" type="xs:string" use="optional"/>
        <xs:attribute name="Suitability" type="xs:string" use="optional"/>
    </xs:complexType>
</xs:schema>
```

B Export File Schema (EXPORT.XSD)

C
Sample Worklist File

This appendix gives an example of a worklist file of the type that would be imported into the Agilent ChemStation. Note that the values contained in this file are not real; they are there only to demonstrate the format.

```
<?xml version="1.0" encoding=" ISO-8859-1"?>
<Samples xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noN-
amespaceSchemaLocation="d:\lego\cpext\txt_imp\xml-templates\worklist.xsd">
    <Sample>
        <Number>1</Number>
        <Location>p1-b1</Location>
        <Name>sample1</Name>
        <CDSMethod>BATCH</CDSMethod>
        <numberOfInj>6</numberOfInj>
        <sampleType>SAMPLE</sampleType>
        <CalLevel>8</CalLevel>
        <calibration>BRACKET</calibration>
        <UpdateRT>NO UPDATE</UpdateRT>
        <Interval>0</Interval>
        <sampleAmount>1</sampleAmount>
        <ISTDAmount>9</ISTDAmount>
        <Multipliers>7</Multipliers>
        <Dilution>7</Dilution>
        <DataFilename>7</DataFilename>
        <InjectionVolume>7</InjectionVolume>
        <description>info</description>
        <StudyName>part 11 demo</StudyName>
        <LimsID>fr37238723</LimsID>
        <LimsKField2>12</LimsKField2>
        <LimsKField3>KF31</LimsKField3>
        <CustomField>
```

```
            <Name>Wish List</Name>
            <Value>3</Value>
        </CustomField>
        <CustomField>
            <Name>Price</Name>
            <Value>5</Value>
        </CustomField>
    </Sample>
    <Sample>
        <Number>2</Number>
        <Location>p1-a1</Location>
        <Name>sample2</Name>
        <CDSMethod>WRONG</CDSMethod>
        <numberOfInj>1</numberOfInj>
        <sampleType/>
        <CalLevel/>
        <calibration/>
        <UpdateRT/>
        <Interval/>
        <sampleAmount>1</sampleAmount>
        <ISTDAmount>2</ISTDAmount>
        <Multipliers>bad</Multipliers>
        <Dilution/>
        <DataFilename>bad</DataFilename>
        <InjectionVolume>bad</InjectionVolume>
        <description>info1</description>
        <StudyName/>
        <LimsID>fr234322</LimsID>
        <LimsKField2>23</LimsKField2>
        <LimsKField3>KF32</LimsKField3>
        <CustomField>
            <Name>Price</Name>
            <Value>6</Value>
        </CustomField>
    </Sample>
</Samples>
```

D
Worklist Schema (WORKLIST.XSD)

This appendix lists the schema that is used to produce the worklist XML file.

```
<?xml version="1.0" encoding=" ISO-8859-1"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" elementFormDe-
fault="qualified" attributeFormDefault="unqualified">
    <xs:element name="Samples">
        <xs:annotation>
            <xs:documentation>worklist for ChemStation sequence import</xs:doc-
umentation>
        </xs:annotation>
        <xs:complexType>
            <xs:sequence>
                <xs:element name="Sample" maxOccurs="unbounded">
                    <xs:complexType>
                        <xs:sequence>
                            <xs:element name="Number" type="xs:integer"/>
                            <xs:element name="Location" type="xs:string"/>
                            <xs:element name="Name" type="xs:string"/>
                            <xs:element name="CDSMethod" type="xs:string"/>
                            <xs:element name="numberOfInj" type="xs:string"/>
                            <xs:element name="sampleType">
                                <xs:simpleType>
                                    <xs:restriction base="xs:string">
                                        <xs:enumeration value="CONTROLSAMPLE"/>
                                        <xs:enumeration value="SAMPLE"/>
                                        <xs:enumeration value="CALIBRATION"/>
                                        <xs:enumeration value="UNKNOWN"/>
                                        <xs:enumeration value="STANDARD"/>
                                        <xs:enumeration value="QUALITYCONTROL"/>
                                        <xs:enumeration value="BLANK"/>
```

```
                <xs:enumeration value="DOUBLEBLANK"/>
                <xs:enumeration value="SOLVENT"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="CalLevel" type="xs:string"/>
    <xs:element name="calibration">
        <xs:simpleType>
            <xs:restriction base="xs:string">
                <xs:enumeration value="NO UPDATE"/>
                <xs:enumeration value="REPLACE"/>
                <xs:enumeration value="BRACKET"/>
                <xs:enumeration value="DELTA%"/>
                <xs:enumeration value="AVERAGE"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="UpdateRT">
        <xs:simpleType>
            <xs:restriction base="xs:string">
                <xs:enumeration value="NO UPDATE"/>
                <xs:enumeration value="REPLACE"/>
                <xs:enumeration value="BRACKET"/>
                <xs:enumeration value="DELTA%"/>
                <xs:enumeration value="AVERAGE"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="Interval" type="xs:string"/>
    <xs:element name="sampleAmount" type="xs:string"/>
    <xs:element name="ISTDAmount" type="xs:string"/>
    <xs:element name="Multipliers" type="xs:string"/>
    <xs:element name="Dilution" type="xs:string"/>
    <xs:element name="DataFilename" type="xs:string"/>
    <xs:element name="InjectionVolume" type="xs:string"/>
    <xs:element name="description" type="xs:string"/>
    <xs:element name="StudyName" type="xs:string"/>
    <xs:element name="LimsID" type="xs:string"/>
```

```
                        <xs:element name="LimsKField2" type="xs:string"/>
                        <xs:element name="LimsKField3" type="xs:string"/>
                        <xs:element name="CustomField" minOccurs="0"
maxOccurs="unbounded">
                            <xs:complexType>
                                <xs:sequence>
                                    <xs:element name="Name" type="xs:string"/>
                                    <xs:element name="Value" type="xs:string"/>
                                </xs:sequence>
                            </xs:complexType>
                        </xs:element>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
</xs:element>
<xs:complexType name="CustomFieldType">
    <xs:sequence>
        <xs:element name="Name" type="xs:string"/>
        <xs:element name="Value" type="xs:string"/>
    </xs:sequence>
</xs:complexType>
</xs:schema>
```

D Worklist Schema (WORKLIST.XSD)

E
XSD File (XMLSchema.xsd)

In this appendix, the schema that is used to produce catalog file generated by the ChemStore is documented.

```
<?xml version="1.0" encoding="UTF-8"?>
<schema targetNamespace="http://www.chem.agi-
lent.com/NDS/ArchiveRestore/XMLSchema"
xmlns="http://www.w3.org/2001/XMLSchema"
xmlns:s="http://www.chem.agilent.com/NDS/ArchiveRe-
store/XMLSchema" elementFormDefault="qualified">
      <annotation>
            <documentation xml:lang="en">Schema for Generic
XML-based Archive/Restore Interface, Copyright Agilent Technolo-
gies, Inc. 2002</documentation>
            <documentation>Version 01.02.03</documentation>
      </annotation>
      <!-- definition of root element (ArchiveCatalog) -->
      <element name="ArchiveCatalog">
            <complexType>
                  <sequence>
                        <element name="Head" type="s:Head-
Type"/>
                        <element name="Body" type="s:Body-
Type"/>
                        <element name="FileProtection" minOc-
curs="0">
                              <complexType>
                                    <sequence>
                                          <element
name="HashValue" type="string"/>
                                    </sequence>
                              </complexType>
```

```
                                    </element>
                              </sequence>
                        </complexType>
                        <keyref name="UserRefs" refer="s:UserKey">
                              <selector xpath=".//s:User"/>
                              <field xpath="s:ID"/>
                              <field xpath="s:Revision"/>
                        </keyref>
                        <key name="UserKey">
                              <selector xpath="s:Body/s:User"/>
                              <field xpath="@ID"/>
                              <field xpath="@Revision"/>
                        </key>
                        <keyref name="InstrumentRefs" refer="s:Instrument-
Key">
                              <selector xpath=".//s:Instrument"/>
                              <field xpath="s:ID"/>
                              <field xpath="s:Revision"/>
                        </keyref>
                        <key name="InstrumentKey">
                              <selector xpath="s:Body/s:Instrument"/>
                              <field xpath="@ID"/>
                              <field xpath="@Revision"/>
                        </key>
                        <keyref name="MethodRefs" refer="s:MethodKey">
                              <selector xpath=".//s:Method"/>
                              <field xpath="s:ID"/>
                              <field xpath="s:Revision"/>
                        </keyref>
                        <key name="MethodKey">
                              <selector xpath="s:Body/s:Method"/>
                              <field xpath="@ID"/>
                              <field xpath="@Revision"/>
                        </key>
                        <keyref name="ProjectRefs" refer="s:ProjectKey">
                              <selector xpath=".//s:Project"/>
                              <field xpath="s:ID"/>
                              <field xpath="s:Revision"/>
                        </keyref>
                        <key name="ProjectKey">
                              <selector xpath="s:Body/s:Project"/>
                              <field xpath="@ID"/>
                              <field xpath="@Revision"/>
```

```
                </key>
                <keyref name="SequenceRefs" refer="s:SequenceKey">
                        <selector xpath=".//s:Sequence"/>
                        <field xpath="s:ID"/>
                        <field xpath="s:Revision"/>
                </keyref>
                <key name="SequenceKey">
                        <selector xpath="s:Body/s:Sequence"/>
                        <field xpath="@ID"/>
                        <field xpath="@Revision"/>
                </key>
        </element>
        <!-- definition of main types (HeadType and BodyType) -->
        <complexType name="HeadType">
                <sequence>
                        <element name="Name" type="string"/>
                        <element name="Description" type="string"/>
                        <element name="Scheduled" type="s:UserDa-
teTimeType" minOccurs="0"/>
                        <element name="Started" type="s:UserDateTime-
Type"/>
                        <element name="Completed" type="s:UserDa-
teTimeType"/>
                        <element name="Computer" type="string" minOc-
curs="0"/>
                        <element name="DirectoryPath" type="string"/>
                        <element name="ArchiveSize" type="string"/>
                        <element name="ProductName" type="string"/>
                        <element name="ProductRevisionNumber"
type="string"/>
                        <element name="DatabaseServerHostName"
type="string"/>
                        <element name="DatabaseServerConnString"
type="string" minOccurs="0"/>
                        <element name="ArchiveContentFromDate"
type="string" minOccurs="0"/>
                        <element name="ArchiveContentEndDate"
type="string" minOccurs="0"/>
                        <element name="ArchiveAndDelete" type="bool-
ean"/>
                        <element name="NumberOfObjectsArchived"
type="unsignedLong" minOccurs="0"/>
                        <element name="ObjectsThatFailedToArchive"
```

```
type="unsignedLong" minOccurs="0"/>
                    <element name="ArchivedQueries" minOc-
curs="0">
                          <complexType>
                                <sequence>
                                      <element name="Query"
type="s:QueryType" maxOccurs="unbounded"/>
                                </sequence>
                          </complexType>
                    </element>
             </sequence>
             <attribute name="ID" type="string"/>
      </complexType>
      <complexType name="BodyType">
             <sequence>
                    <element name="User" type="s:UserType" minOc-
curs="0" maxOccurs="unbounded"/>
                    <element name="Instrument" type="s:Instru-
mentType" minOccurs="0" maxOccurs="unbounded"/>
                    <element name="Method" type="s:MethodType"
minOccurs="0" maxOccurs="unbounded"/>
                    <element name="Project" type="s:ProjectType"
minOccurs="0" maxOccurs="unbounded"/>
                    <element name="Sequence" type="s:Sequence-
Type" minOccurs="0" maxOccurs="unbounded"/>
                    <element name="Sample" type="s:SampleType"
minOccurs="0" maxOccurs="unbounded"/>
             </sequence>
      </complexType>
      <!-- definition of "HeadType" types -->
      <complexType name="QueryType">
             <sequence>
                    <element name="Name" type="string"/>
                    <element name="CannedQueryName" type="string"
minOccurs="0"/>
                    <element name="FilterAttributesSpecifiedBy-
User" type="string" minOccurs="0"/>
             </sequence>
      </complexType>
      <!-- definition of "BodyType" types -->
      <complexType name="UserType">
             <complexContent>
                    <extension base="s:SimpleObjectType"/>
```

```
            </complexContent>
      </complexType>
      <complexType name="InstrumentType">
            <complexContent>
                  <extension base="s:SimpleObjectType">
                        <sequence>
                              <element name="Technique"
type="string" minOccurs="0"/>
                        </sequence>
                  </extension>
            </complexContent>
      </complexType>
      <complexType name="MethodType">
            <complexContent>
                  <extension base="s:SimpleObjectType">
                        <sequence>
                              <element name="Quantification-
Method" type="string" minOccurs="0"/>
                              <element name="Instrument"
type="s:NameOrObjectRefType" minOccurs="0"/>
                        </sequence>
                  </extension>
            </complexContent>
      </complexType>
      <complexType name="ProjectType">
            <complexContent>
                  <extension base="s:SimpleObjectType"/>
            </complexContent>
      </complexType>
      <complexType name="SequenceType">
            <complexContent>
                  <extension base="s:SimpleObjectType"/>
            </complexContent>
      </complexType>
      <complexType name="SampleType">
            <complexContent>
                  <extension base="s:SimpleObjectType">
                        <sequence>
                              <element name="Type"
type="string"/>
                              <element name="Category"
type="string" minOccurs="0"/>
                              <element name="BarCode"
```

```
type="string" minOccurs="0"/>
                                    <element name="LimsID"
type="string" minOccurs="0"/>
                                    <element name="CalibLevel"
type="unsignedLong" minOccurs="0"/>
                                    <element name="ProductCode"
type="string" minOccurs="0"/>
                                    <element name="Acquisition"
type="s:AcquisitionType" minOccurs="0"/>
                                    <element name="Result"
type="s:ResultType" minOccurs="0" maxOccurs="unbounded"/>
                              </sequence>
                        </extension>
                  </complexContent>
            </complexType>
            <!-- definition of "BodyType" child types -->
            <complexType name="AcquisitionType">
                  <complexContent>
                        <extension base="s:NonVersionedObjectType">
                              <sequence>
                                    <element name="Sequence"
type="s:NameOrObjectRefType" minOccurs="0"/>
                                    <element name="Method"
type="s:AcquisitionMethodType" minOccurs="0"/>
                                    <element name="Instrument"
type="s:NameOrObjectRefType" minOccurs="0"/>
                                    <element name="RawData"
type="s:RawDataType" minOccurs="0" maxOccurs="unbounded"/>
                              </sequence>
                        </extension>
                  </complexContent>
            </complexType>
            <complexType name="ResultType">
                  <complexContent>
                        <extension base="s:NonVersionedObjectType">
                              <sequence>
                                    <element name="Sequence"
type="s:NameOrObjectRefType" minOccurs="0"/>
                                    <element name="Project"
type="s:NameOrObjectRefType" minOccurs="0"/>
                                    <element name="Method"
type="s:NameOrObjectRefType" minOccurs="0"/>
                                    <element name="Compounds" minOc-
```

```
curs="0">
                                          <complexType>
                                                <sequence>
                                                      <element
name="Compound" type="s:CompoundType" minOccurs="0" maxOc-
curs="unbounded"/>
                                                </sequence>
                                          </complexType>
                                    </element>
                                    <element name="CustomFields"
minOccurs="0">
                                          <complexType>
                                                <sequence>
                                                      <element
name="CustomField" type="s:CustomFieldType" minOccurs="0" maxOc-
curs="unbounded"/>
                                                </sequence>
                                          </complexType>
                                    </element>
                                    <element name="Approval"
type="s:ApprovalType" minOccurs="0"/>
                              </sequence>
                        </extension>
                  </complexContent>
            </complexType>
            <!-- definition of "BodyType" grand-child types -->
            <complexType name="RawDataType">
                  <complexContent>
                        <extension base="s:NonVersionedObjectType">
                              <sequence>
                                    <element name="Computer"
type="string" minOccurs="0"/>
                                    <element name="DirectoryPath"
type="string" minOccurs="0"/>
                                    <element name="Signals" minOc-
curs="0">
                                          <complexType>
                                                <sequence>
                                                      <element
name="Channel" type="s:ChannelType" minOccurs="0" maxOc-
curs="unbounded"/>
                                                </sequence>
                                          </complexType>
```

```
                                        </element>
                                  </sequence>
                            </extension>
                      </complexContent>
               </complexType>
               <complexType name="ChannelType">
                      <sequence>
                            <element name="Name" type="string"/>
                            <element name="Type" type="string"/>
                      </sequence>
               </complexType>
               <complexType name="CompoundType">
                      <sequence>
                            <element name="Name" type="string"/>
                            <element name="RT" type="string"/>
                            <element name="CorrectedRT" type="string"/>
                            <element name="Height" type="string"/>
                            <element name="Area" type="string"/>
                            <element name="AreaPercentage"
type="string"/>
                            <element name="Amount" type="string"/>
                            <element name="RF" type="string"/>
                      </sequence>
               </complexType>
               <complexType name="CustomFieldType">
                      <sequence>
                            <element name="Name" type="string"/>
                            <element name="Value">
                                  <complexType>
                                        <simpleContent>
                                              <extension base="string">
                                                    <attribute
name="Type" type="string"/>
                                              </extension>
                                        </simpleContent>
                                  </complexType>
                            </element>
                            <element name="Unit" type="string" minOc-
curs="0"/>
                      </sequence>
               </complexType>
               <complexType name="CustomFieldValueType"/>
               <complexType name="ApprovalType">
```

```
            <complexContent>
                  <extension base="s:UserDateTimeType">
                        <sequence>
                              <element name="Description"
type="string" minOccurs="0"/>
                              <element name="Status"
type="string" minOccurs="0"/>
                        </sequence>
                  </extension>
            </complexContent>
      </complexType>
      <!-- definition of reference (or simple) types -->
      <complexType name="AcquisitionMethodType">
            <choice>
                  <sequence>
                        <element name="ID" type="string"/>
                        <element name="Revision" type="unsign-
edLong"/>
                  </sequence>
                  <sequence>
                        <element name="Name" type="string"/>
                        <element name="Modified" type="s:User-
DateTimeType" minOccurs="0"/>
                  </sequence>
            </choice>
      </complexType>
      <complexType name="NameOrObjectRefType">
            <choice>
                  <sequence>
                        <element name="ID" type="string"/>
                        <element name="Revision" type="unsign-
edLong"/>
                  </sequence>
                  <sequence>
                        <element name="Name" type="string"/>
                  </sequence>
            </choice>
      </complexType>
      <complexType name="ObjectRefType">
            <sequence>
                  <element name="ID" type="string"/>
                  <element name="Revision" type="unsigned-
Long"/>
```

```
            </sequence>
      </complexType>
      <!-- definition of other types -->
      <complexType name="SimpleObjectType">
            <complexContent>
                  <extension base="s:NonVersionedObjectType">
                        <sequence>
                              <element name="Modified"
type="s:UserDateTimeType" minOccurs="0"/>
                              <element name="Status"
type="string" minOccurs="0"/>
                        </sequence>
                  </extension>
            </complexContent>
      </complexType>
      <complexType name="NonVersionedObjectType">
            <sequence>
                  <element name="Name" type="string"/>
                  <element name="Description" type="string"
minOccurs="0"/>
                  <element name="Created" type="s:UserDateTime-
Type" minOccurs="0"/>
            </sequence>
            <attribute name="ID" type="string" use="required"/>
            <attribute name="Revision" type="unsignedLong"
use="required"/>
      </complexType>
      <complexType name="UserDateTimeType">
            <sequence>
                  <element name="User" type="s:NameOrObjec-
tRefType"/>
                  <element name="DateTime" type="dateTime"/>
            </sequence>
      </complexType>

</schema>
```

F
Example XML file (XMLSchema_example.xml)

Example XML file (XMLSchema_example.xml)

```
<?xml version="1.0" encoding="UTF-8" ?>
<ArchivingCatalog xmlns="http://www.chem.agi-
    lent.com/NDS/ArchiveRestore/XMLSchema"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="http://www.chem.agilent.com/NDS/ArchiveR-
    estore/XMLSchema XMLSchema.xsd">
  <Head>
    <Name>Archive_20020923A</Name>
    <Description>manually created example archive cata-
        log</Description>
    <Started>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
      <DateTime>2002-09-23T14:15:00</DateTime>
    </Started>
    <Completed>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
      <DateTime>2002-09-23T14:30:59</DateTime>
```

```
    </Completed>
    <Computer>csserver.agilent.com</Computer>
    <DirectoryPath>f:\ChemStore_Archives</DirectoryPath>
    <ArchiveSize>100000</ArchiveSize>
    <ProductName>Agilent ChemStore C/S</ProductName>
    <ProductRevisionNumber>B.02.02</ProductRevisionNumber>
    <DatabaseServerHostName>csserver.agilent.com</DatabaseServer-
    HostName>
    <ArchiveAndDelete>false</ArchiveAndDelete>
</Head>
<Body>
    <User ID="0" Revision="0">
      <Name>internal</Name>
      <Description>this is an internal ChemStore user</Descrip-
          tion>
    </User>
    <User ID="1" Revision="0">
      <Name>admin</Name>
      <Description>Administrator</Description>
      <Created>
        <User>
          <ID>0</ID>
          <Revision>0</Revision>
        </User>
        <DateTime>2002-09-23T11:40:00</DateTime>
      </Created>
      <Modified>
        <User>
          <ID>1</ID>
          <Revision>0</Revision>
        </User>
        <DateTime>2002-09-23T11:41:00</DateTime>
```

```
    </Modified>
    <Status>Active</Status>
</User>
<Instrument ID="101" Revision="0">
    <Name>example instrument</Name>
    <Modified>
      <User>
        <Name />
      </User>
      <DateTime>2002-09-23T11:45:00</DateTime>
    </Modified>
</Instrument>
<Method ID="201" Revision="0">
    <Name>example method</Name>
    <Description>this is my favorite method</Description>
    <Modified>
      <User>
        <Name />
      </User>
      <DateTime>2002-09-23T11:50:00</DateTime>
    </Modified>
    <QuantificationMethod>Area Pct</QuantificationMethod>
</Method>
<Project ID="301" Revision="0">
    <Name>example project</Name>
    <Description>this is my favorite study, infact it's the
        only one ;-)</Description>
    <Created>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
```

```
      <DateTime>2002-09-23T11:30:00</DateTime>
    </Created>
    <Modified>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
      <DateTime>2002-09-23T11:31:01</DateTime>
    </Modified>
    <Status>Active</Status>
  </Project>
  <Sequence ID="401" Revision="0">
    <Name>example sequence</Name>
    <Description>this is my favorite sequence</Description>
    <Modified>
      <User>
        <Name />
      </User>
      <DateTime>2002-09-23T11:56:58</DateTime>
    </Modified>
  </Sequence>
  <Sample ID="501" Revision="0">
    <Name>example sample</Name>
    <Created>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
      <DateTime>2002-09-23T13:14:15</DateTime>
    </Created>
    <Type>Sample</Type>
    <Acquisition ID="601" Revision="0">
```

```
<Name />
<Created>
   <User>
      <ID>1</ID>
      <Revision>0</Revision>
   </User>
   <DateTime>2002-09-23T13:14:15</DateTime>
</Created>
<Sequence>
   <Name>sequence.s</Name>
</Sequence>
<Method>
   <Name>LCmethod.m</Name>
   <Modified>
      <User>
         <Name />
      </User>
      <DateTime>2002-09-23T12:13:14</DateTime>
   </Modified>
</Method>
<Instrument>
   <ID>101</ID>
   <Revision>0</Revision>
</Instrument>
<RawData ID="701" Revision="0">
   <Name>MIX00003.D</Name>
   <Description>this is an example data file</Descrip-
       tion>
   <Created>
      <User>
         <Name />
      </User>
```

```
        <DateTime>2002-09-23T12:15:16</DateTime>
      </Created>
      <Computer>PC123456</Computer>
      <DirectoryPath>C:\CHEM32\1\data</DirectoryPath>
      <Signals>
        <Channel>
          <Name>DAD 1A, Sig=254,4 Ref=550,100</Name>
          <Type>Absorbance</Type>
        </Channel>
      </Signals>
    </RawData>
  </Acquisition>
  <Result ID="801" Revision="1">
    <Name />
    <Created>
      <User>
        <ID>1</ID>
        <Revision>0</Revision>
      </User>
      <DateTime>2002-09-23T12:33:33</DateTime>
    </Created>
    <Sequence>
      <ID>401</ID>
      <Revision>0</Revision>
    </Sequence>
    <Project>
      <ID>301</ID>
      <Revision>0</Revision>
    </Project>
    <Method>
      <ID>201</ID>
      <Revision>0</Revision>
```

```
      </Method>
      <Compounds>
        <Compound>
          <Name>Biphenyl</Name>
          <RT>2.56547093391418</RT>
          <CorrectedRT>2.5661883381983</CorrectedRT>
          <Height>26.8392372131348</Height>
          <Area>176.11506652832</Area>
          <Amount>5.99505058242023E-03</Amount>
          <RF>3.40405321395725E-05</RF>
        </Compound>
      </Compounds>
      <CustomFields>
        <CustomField>
          <Name>Temperature</Name>
          <Value Type="real">21.1</Value>
          <Unit>°C</Unit>
        </CustomField>
      </CustomFields>
      <Approval>
        <User>
          <ID>1</ID>
          <Revision>0</Revision>
        </User>
        <DateTime>2002-09-23T12:34:56</DateTime>
        <Description>I think that I can approve this
            run.</Description>
        <Status>Approved</Status>
      </Approval>
    </Result>
</Sample>
<Sample ID="502" Revision="0">
```

```
<Name>Sample 2</Name>
<Created>
  <User>
    <ID>1</ID>
    <Revision>0</Revision>
  </User>
  <DateTime>2002-09-23T13:15:16</DateTime>
</Created>
<Type>Sample</Type>
<Acquisition ID="602" Revision="0">
  <Name />
  <Sequence>
    <Name>sequence.s</Name>
  </Sequence>
  <Method>
    <Name>LCmethod.m</Name>
    <Modified>
      <User>
        <Name />
      </User>
      <DateTime>2002-09-23T12:13:14</DateTime>
    </Modified>
  </Method>
  <Instrument>
    <ID>101</ID>
    <Revision>0</Revision>
  </Instrument>
  <RawData ID="701" Revision="0">
    <Name>MIX00004.D</Name>
    <Description />
    <Created>
      <User>
```

```
            <Name />
          </User>
          <DateTime>2002-09-23T12:16:16</DateTime>
        </Created>
        <Computer>PC123456</Computer>
        <DirectoryPath>C:\CHEM32\1\data</DirectoryPath>
        <Signals>
          <Channel>
            <Name>DAD 1A, Sig=254,4 Ref=550,100</Name>
            <Type>absorbance</Type>
          </Channel>
        </Signals>
      </RawData>
    </Acquisition>
    <Result ID="802" Revision="3">
      <Name />
      <Created>
        <User>
          <ID>1</ID>
          <Revision>0</Revision>
        </User>
        <DateTime>2002-09-23T12:33:35</DateTime>
      </Created>
      <Sequence>
        <ID>401</ID>
        <Revision>0</Revision>
      </Sequence>
      <Project>
        <ID>301</ID>
        <Revision>0</Revision>
      </Project>
      <Method>
```

```
            <ID>201</ID>
            <Revision>0</Revision>
          </Method>
        </Result>
      </Sample>
    </Body>
    <FileProtection>
      <HashValue>L8nkLEAz8xDfGPAwHHl.zXx7</HashValue>
    </FileProtection>
  </ArchivingCatalog>
```

Special Formatting:

- Body Objects (located directly under <Body>) appear green.
- References to Body Objects (consisting of ID and Revision) appear blue.
- Embedded Body Objects (types that could also be located directly under <Body>) appear orange.
- Embedded Sample Objects (located directly under <Sample>) appear brown.

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In This Book

This Guide describes the implementation of the XML interface between the Agilent ChemStation Plus and a LIMS system. It also contains examples of import and export XML files, as well as their associated schemas.

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Printed in Germany
05/2005

G2170-90223

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